Charge and Light Production Modeling at Low Energy

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Tuesday December 1, 2020 LEPLAr Workshop

What is NEST?

Fully integrated into Geant4 and Garfield++. Other languages: Python, ROOT

- Noble Element Simulation Technique: it's neutral and impartial, open-source
- A non-partisan, inter-collaboration collaboration with representatives from XENON1T/nT/DARWIN, LUX/LZ, (n)EXO, RED, DUNE, SBN, MicroBooNE, and COHERENT!
- Name also of the software, which does LXe, GXe, SXe, and LAr (very preliminary testing stage)
- Primary parameters: particle or interaction type, E-fields, density or phase, and energy or dE/dx (latter more critical for MeV to GeV scale energies: ER)
- Reduce your systematics by relying not only on your own calibration data, but upon all of those who came before you. Stop reinventing the wheel, with "NEST-like" but proprietary software
- Snowmass LOI to multiple frontiers: 100+ authors, >40 institutions across 4 continents. DUNE and DarkSide represented

https://www.snowmass21.org/docs/files/summaries/IF/SNOWMASS21-IF8_IF0-NF5_NF10-CF1_CF0-CompF5_CompF7_Matthew_Szydagis-104.pdf

Get the full code here, from GitHub
https://github.com/NESTCollaboration/nest

And, What Can It Simulate?

- Monte Carlo capabilities: growing all of the time, with multiple options like Geant4
- Mean scintillation light and ionization (charge) yields versus parameters earlier
- Energy resolution: the width in those yields, and their skewness
- BG discrimination: leakage of events into signal region (e.g. WIMPs/e-, e-/gamma)
- Pulse timing profiles, including widths and general shapes: both primary and secondary scintillation
- Built-in calculation of the efficiency or threshold, and the log(S2) or S2/S1 band means & widths
- *Basic spin-independent and spin-dependent WIMP limit calculator (Feldman-Cousins)*
- Detector effects like photon detection < 100%, on top of detector-independent aspects like yields
- Noise: correlated, anti-correlated, and uncorrelated sources all simulated now

The Institutions Represented Right Now on NEST

nest.physics.ucdavis.edu

UNIVERSITY AT ALBANY
State University of New York

(me!)

UC DAVIS

Rensselaer

Berkeley
UNIVERSITY OF CALIFORNIA

ITEP

MEPhI

RICE

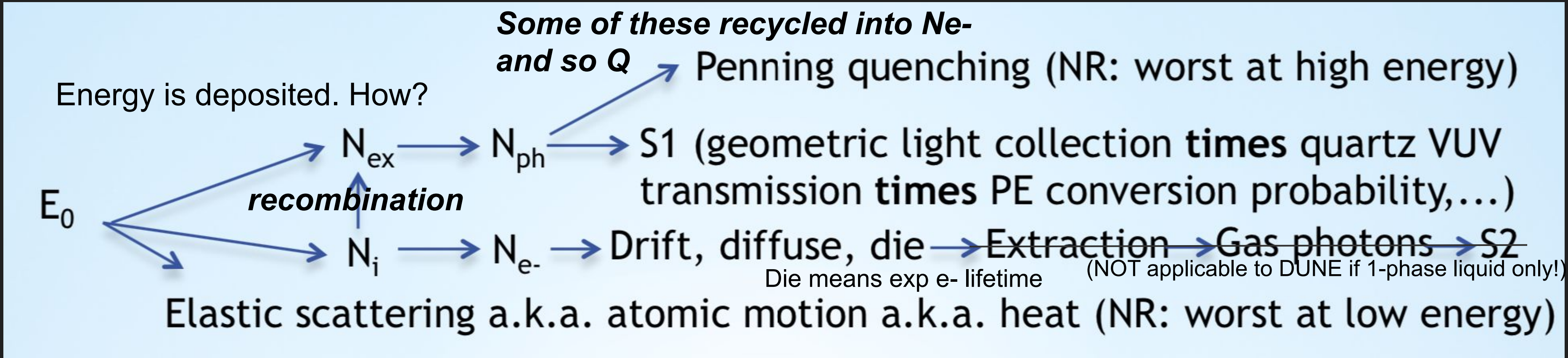
Lawrence Livermore National Laboratory

Unfunded, but still REAL collaboration!

UC San Diego

Colorado State University

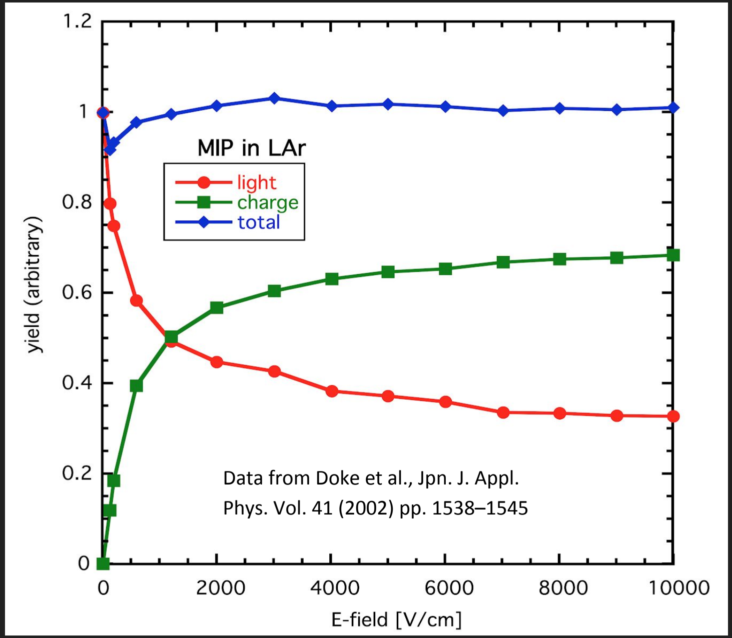
The Microphysics of Energy Partitioning: Not Trivial!



- Chain reaction set off by 1 NR (nuclear recoil) or 1 ER (electron recoil) leads to many NRs and ERs, with 3 primary processes occurring
  - Elastic ("billiard-ball") scattering or inelastic: electron excitation and ionization
- Almost every arrow above is energy-dependent and many electric field-dependent
- NEST also comes with all the trimmings: for instance, e- drift speed & diffusion
  - Singlet/triplet t's considered, not ignored as in above simplified diagram. (Also, extraction efficiency)

Anti-Correlation is a Real Effect in LAr, just as in LXe

- Charge is only ~half of the story for energy
  - For low energies, and high enough scintillation photon detection efficiency, it does become more important, when you don't have a massive and healthy Q signal
  - For dark matter, light alone was thought to be energy!
- Fun fact: I was on DUNE (LBNE at time) but only briefly, as Bob Svoboda's postdoc at UCD and you can find original version of this plot somewhere in old LBNE docdb, if it still exists?
  - Find all my old analyses searching my last name :)
- This was shown more recently by LArIAT using Michel electrons. See arXiv:1909.07920
  - Recombination fluctuations become canceled out: see Conti et al. 2003: arXiv:hep-ex/0303008 (liquid Xenon)
  - Fano factor is sub-Poissonian on the total quanta



Our own re-analysis of Doke et al. 2002. A 976 keV electron paired with 1.05 MeV gamma ray, very low energies, but could still be relevant -- at least at this workshop!

Quantifying the LEP Benefit

g_1 [%]	0% Q noise	1%	2%	5%	10%	20%	50%	100%
0.001 (10^-5)	0.46	1.10	2.05	4.99	10.0	20.1	46.0	62.5
0.002	0.46	1.10	2.05	4.99	10.0	20.1	46.0	62.5
0.005	0.46	1.10	2.05	4.99	10.0	20.1	46.0	54.6
0.01	0.46	1.10	2.05	4.99	10.0	20.1	40.5	46.6
0.02	0.46	1.10	2.05	4.99	10.0	20.1	34.1	42.4
0.05	0.46	1.10	2.05	4.99	10.0	17.8	28.9	31.5
0.1	0.46	1.10	2.05	4.99	10.0	14.5	22.1	22.1
0.2	0.46	1.10	2.05	4.99	8.78	12.7	15.6	15.6
0.5	0.46	1.10	2.05	4.99	7.12	10.0	10.0	10.0
1	0.46	1.10	2.05	4.21	6.34	7.08	7.08	7.08
2	0.46	1.10	2.05	3.55	4.99	4.99	4.99	4.99
5	0.46	1.10	1.79	3.08	3.14	3.14	3.14	3.14
10	0.46	1.10	1.47	2.20	2.20	2.20	2.20	2.20
20	0.46	0.87	1.28	1.53	1.53	1.53	1.53	1.53
50	0.39	0.67	0.91	0.91	0.91	0.91	0.91	0.91
100	0.21	0.57	0.57	0.57	0.57	0.57	0.57	0.57

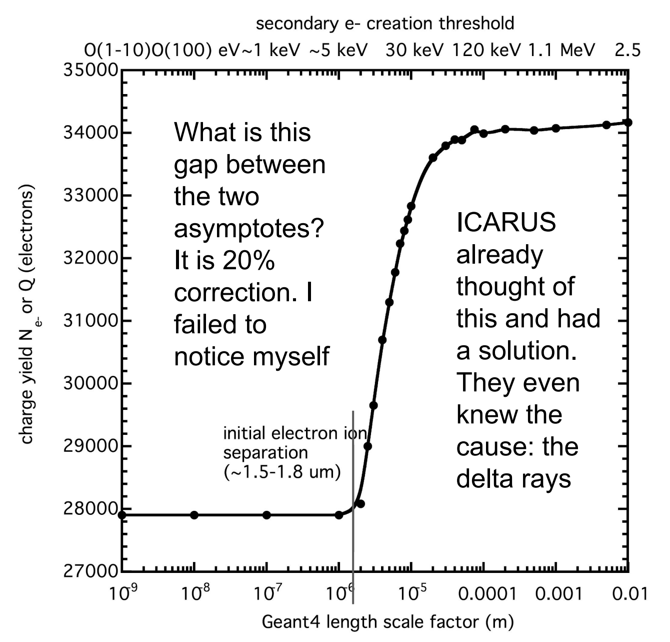
Estimated lowest resolution of 1 MeV electron recoil at 0.5 kV/cm, as a function of g_1 and wire noise. Note that this is a simplified example, since a stand-alone simulation without Geant4. Delta rays may change the story: if anything, making combined-energy scale and/or S1-only even better than Q-only than shown

- The bad news is that it will take a large g_1 (primary scintillation photon detection efficiency) to benefit
- See the table at left, from our upcoming energy recon/res review paper in the journal *Instruments*
  - You should be able to find old (Geant4) versions of table by me for 50, 500 MeV
- Resolution in a DUNE-like detector can be halved already at g1 = 2% (0.02) for 10% Q noise on the wires
  - Orders of magnitude higher than planned, but far smaller than achieved in DM experiments already. Doable?
- Table mixes the Q-only, combined, and even S1-only energy scales

Yield Breakdown: Delta Rays Key

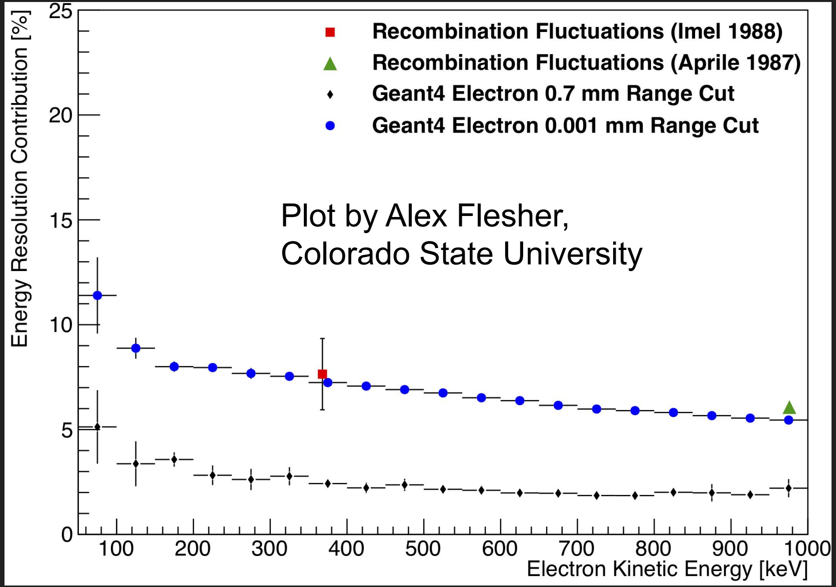
- You get wrong charge (and light) yield if you don’t produce enough of them at low energies
  - Because of secondary particle production, this isn’t a problem at only low energies, however
- How was this taken into account in the past?
  - This is the 0.8 correction in the **ICARUS** Birks Law model! (Amoruso et al. 2003/2004) Box model in use now probably has a similar offset effectively
- G4 doesn’t go down to 1-nm scale (~100 eV) for electrons, but we know left asymptote is right based on Doke data, couple slides ago
  - Another factoid: e^--ion separation (Mozumder 1995)
- Why does this happen?
  - Delta rays are low-energy, high-dE/dx: more light, less charge, so more charge if they are not in sim

1 MeV at 500 V/cm field once again. “Infinite” LAr volume in a stand-alone Geant4 simulation. No charge loss or wire noise simulated here. Default cut-off in LArSoft? It’s way too high...



This is the ArgoNeuT modified Thomas-Imel box model in LArSoft, not Birks Law even. This is not a problem with one model, or one software, or one energy range. It is a universal issue

500 V/cm again, but varying energy



1 Correction is Not Sufficient

- This is new: one can't just renormalize mean yield and be done with it -- because the widths are affected as well
  - Probably ugly energy/field-dependent kludge
- You can't reproduce the resolution in real data (Thomas, Imel, & Biller and Aprile, 1987-1988) without O(10 keV) delta rays
  - Doing O(100 keV) is not going to cut it
- Surely worth slower sim time for precision
  - Perhaps not big part of whole? Supercomputing
- Additional trick: combined-E scale will help, because recombination fluctuations from delta rays should be "absorbed"

back to mean yields from widths: how to model them

- You are all familiar with this formulation, of Birks' Law from ICARUS in 2003, except maybe not with all of the terms (Q_y is = to Q or N_{e-} per energy, or dQ/dE)

$$Q_y(\frac{dE}{dx},\mathcal{E}) = A\frac{1/W_i}{1+(k_B/\mathcal{E})(dE/dx)} = A\frac{Q_0(E)/E}{1+(k_B/\mathcal{E})(dE/dx)}$$

https://doi.org/10.1016/j.nima.2003.11.423 has been the guiding principle for NEST.

- But in 2012-13, we had suggested this instead, closer to first principles, as done in LXe experiments, plus LAr-based ones for dark matter:

$$E = N_q W_q = (N_{ph} + N_{e-})W_q \text{ where } N_{ph} = N_{ex} + r(E,\mathcal{E})N_i \text{ and } N_{e-} = [1 - r(E,\mathcal{E})]N_i$$

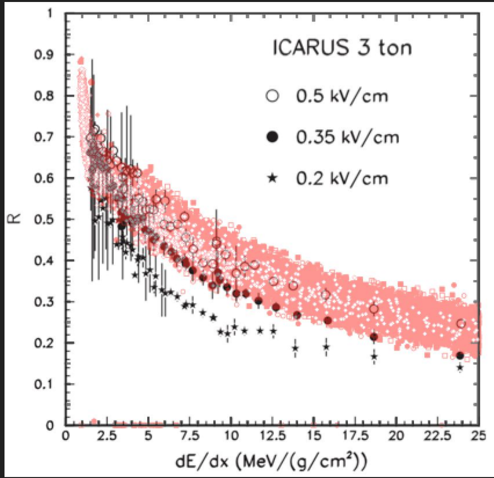
$$r(E,\mathcal{E}) = \frac{k(\mathcal{E})dE/dx}{1+k(\mathcal{E})dE/dx},\quad N_{e-} = (1-r)N_i \rightarrow \frac{N_{e-}}{E} = Q_y = (1-r)\frac{N_i}{E} = \frac{1-r}{W_i} = \frac{1/W_i}{1+k(\mathcal{E})dE/dx}$$

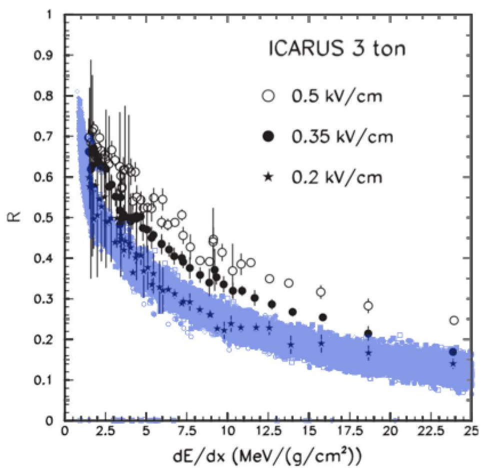
- Using the same steps as followed by the 2011 NEST paper, you get back the same Birks equation, except without that A (0.8, which you don't need anyway)
- What is W_q? More fundamental than W_i: $W_i = (1+0.21)W_q = 1.21 * (19.5 \text{ eV}) = 23.6 \text{ eV},$

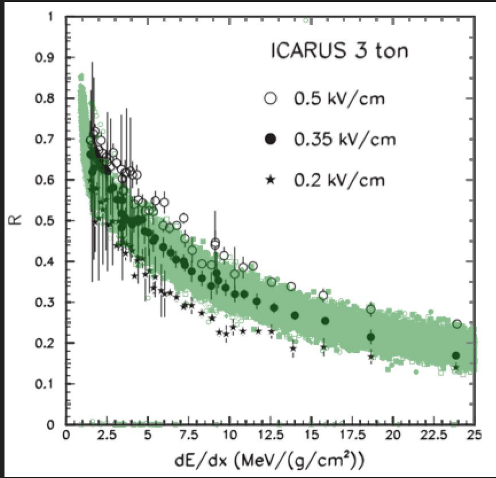
How does such an approach fare against the real data?

$$Q = (1-r)N_i \rightarrow R = 1 - r = Q/N_i = QW_i/E$$

(to clear up any confusion on small ‘r’ versus big ‘R’)

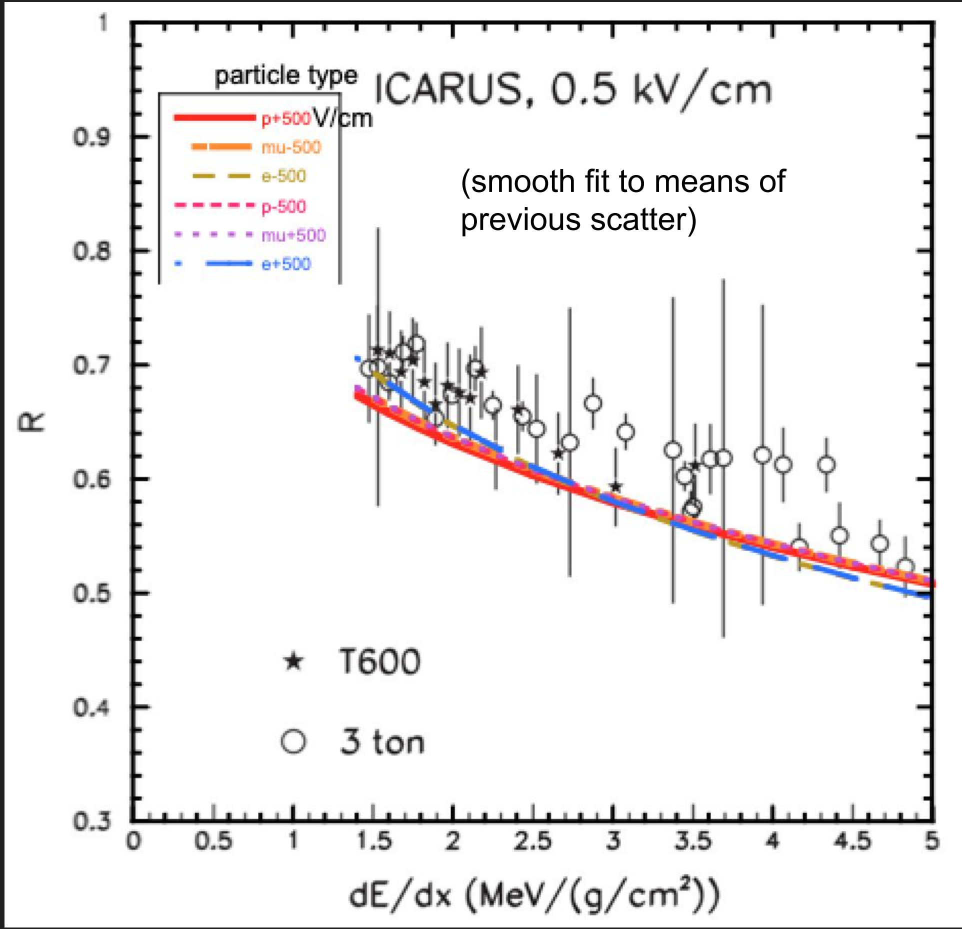






- R = 1-r vs. dE/dx at 3 fields: NEST 2013 LAr model (secondary option in LArSoft at time) in red, green, blue with decreasing E-field from left to right. Solid circles p+, squares mu-, diamonds e-, with antiparticles hollow. $k(\mathcal{E}) = 0.07/\mathcal{E}^{0.85}$ Power < 1, but identical to https://ieeexplore.ieee.org/document/1490090

Not So Great at Low LET

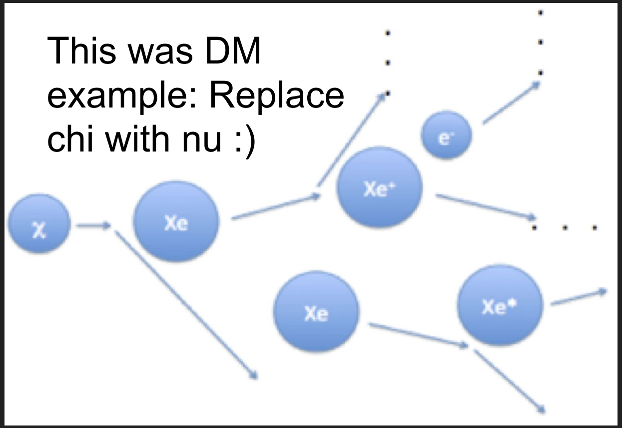


- Bummer, since low dE/dx or LET most important in neutrino physics
- But, that is OK: future work (CSU)
  - Grand synthesis of Birks and Box model's best features underway, with delta rays fully turned ON in G4
  - Birks better at low dE/dx and high energy, but Box at high dE/dx and low energy (as it was for xenon)
- Preliminary new LAr model is in latest NEST (v2.2.0) but not ready for prime time yet (please wait)
  - In there mainly for DM, CEvNS (NR)
- Nevertheless, important: e- curve not necessarily same as p+, mu-

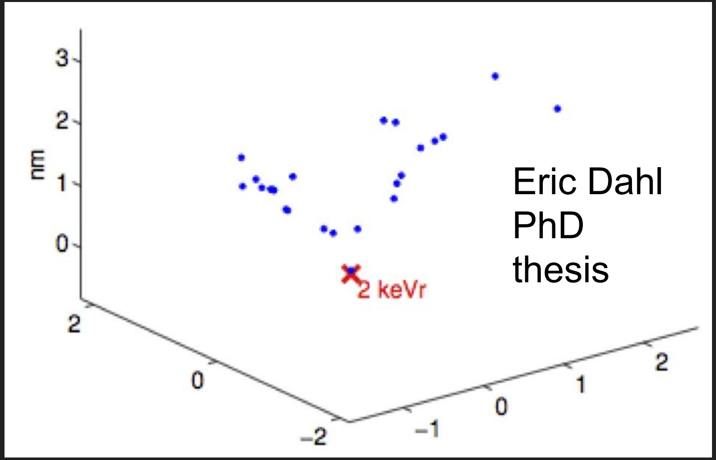
So, where are we going next with NEST for LAr?

- Semi-empirical approach: don’t be married to Birks or Box if data too precise
    - This happened in liquid xenon: the first principles approaches eventually broke down
    - https://docs.google.com/document/d/1vLg8vvY5bcdl4Ah4fzyE182DGWt0Wr7_FJ12_B10ujU
- Merging of all relevant LAr data from dark matter detectors: there are many that should not be ignored: DarkSide, ArDM (2-phase, non-zero-field); DEAP, CLEAN (1-phase, but 0 V/cm). Use low-delta-ray (low-E) data for validation
    - Because of delta rays and other secondary particles, and also renewed interest in LEP, their data is not irrelevant. Cross-fertilization is possible, and is already underway within NEST
    - Great re-fit is underway, in dE/dx basis, of all data from LET of 1.5 up to ~100 MeV*cm^2/g ! from zero electric field out to a few kV/cm. Electrons, gammas, protons, and muons
- Other particles are not forgotten: NEST already does alphas well, since 2012
    - See plots, for neutrons too, at: http://nest.physics.ucdavis.edu/benchmark-plots-argon
- Other effects not in there right now will be added, like separation of geminate (early) recombination mentioned by Doke and others over the decades

What is the Long-Term Future?



- For extrapolation where no data, go fully "theoretical": molecular dynamics simulations
  - Simulate van der Waals forces between the Xe and Ar atoms in liquid, with e.g. 12-6 Lennard-Jones potential from chemistry and atomic physics. Can do DOPING
  - Do optical photon tracking, instead of relying on G4, which is volume instead of surface-based, very slow
- Need to interest funding agencies, like the DOE and the NSF: Snowmass right place?
  - No success in half a decade in securing funds for this
  - Interdisciplinary in full sense of word: beyond HEP. We require AMO expertise.
- Massive supercomputing resources will be needed to simulate many picosec-sized steps
  - But, ironically, lower energies easier: fewer atoms



- Knowing me, I will be very much running out of time before I reach this slide...

Summary/Outlook: Do Combined-E, & Delta Rays!

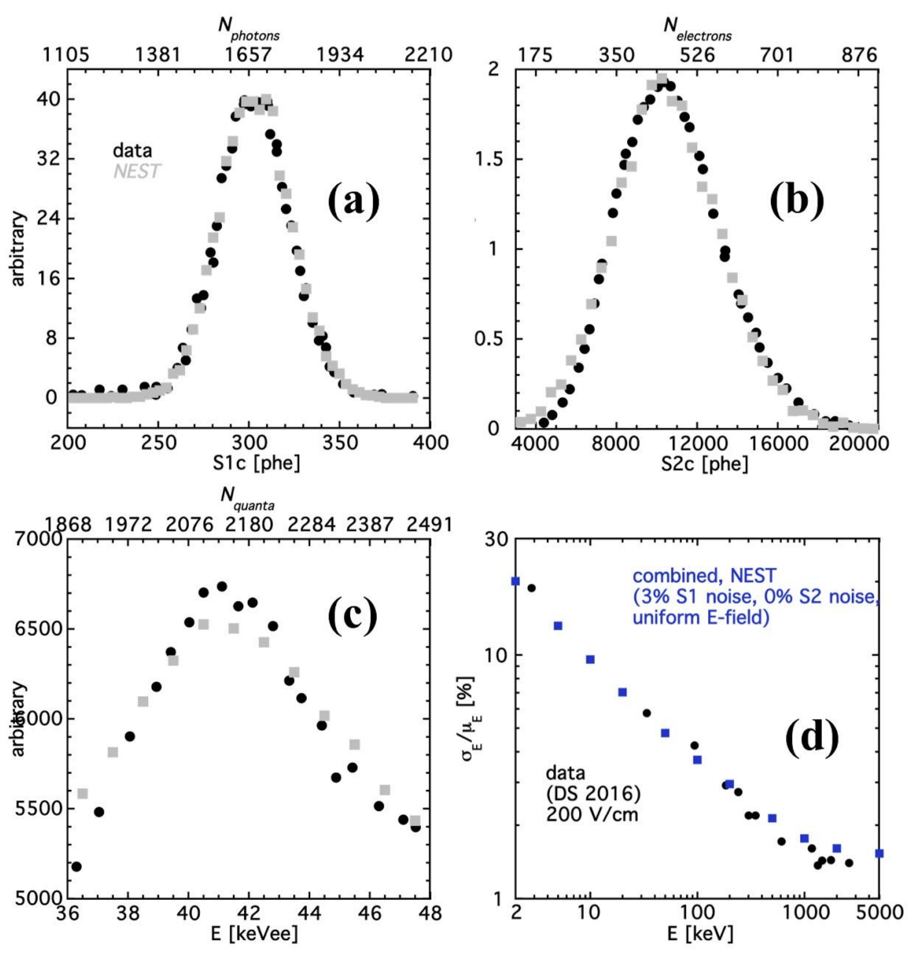
- NEST is quite robust, balancing not just theory and experiment, but also speed (at GeV scale can still simulate thousands of event/min) and precision
  - Allows you to extrapolate not just interpolate, and predict not just postdict data
  - Splits general phenomena from detector idiosyncrasies, but does not ignore the latter
- Constantly being updated, but also being careful to avoid ambulance chasing
  - Minor releases ~monthly, major ~bi-annual. Continuous integration with Travis
- Most important conclusion: NEST works for both Xenon (liquid & gas) and Argon, using similar (often identical) equations/formulae/functions
  - Has in 10 years reduced MC errors (~100% to 10%) incorporating always the world-leading calibrations from ANY experiment. Not restricted to LUX and LZ, where NEST started
  - High speed allows you to train machine learning very fast for detectors using these elements
- Allows you to extract efficiency from PE/keV -> photons, electrons / keV!
  - Excellent for comparing between experiments. Good for theorists and phenomenologists

More References

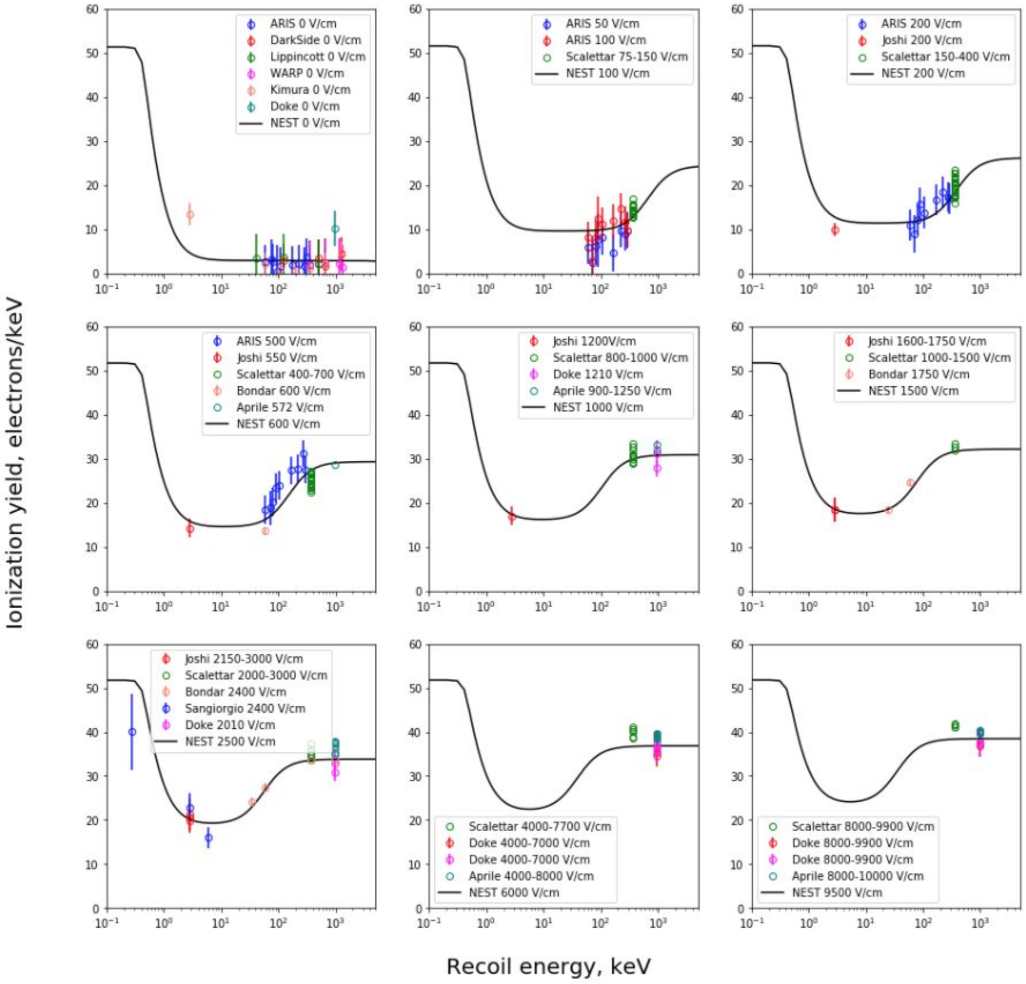
- Cite us using Zenodo: https://zenodo.org/record/4283077#.X8Uqsi2ZO8o
  - Version 2.2.0 has just been tagged, with many bug fixes and lots of new features!
  - You get a fully citable DOI for your publications. Reproducibility, history
- NEST papers (4 so far) listed here: http://nest.physics.ucdavis.edu
  - All old talks listed here as well for download, and various pre-publication analysis reports
  - Validation plots, and online calculator (means only, outdated: better to just download the code)

- See numerous relevant papers by others cited throughout this talk
- Multiple new NEST papers coming as well, really big ones! Be on lookout

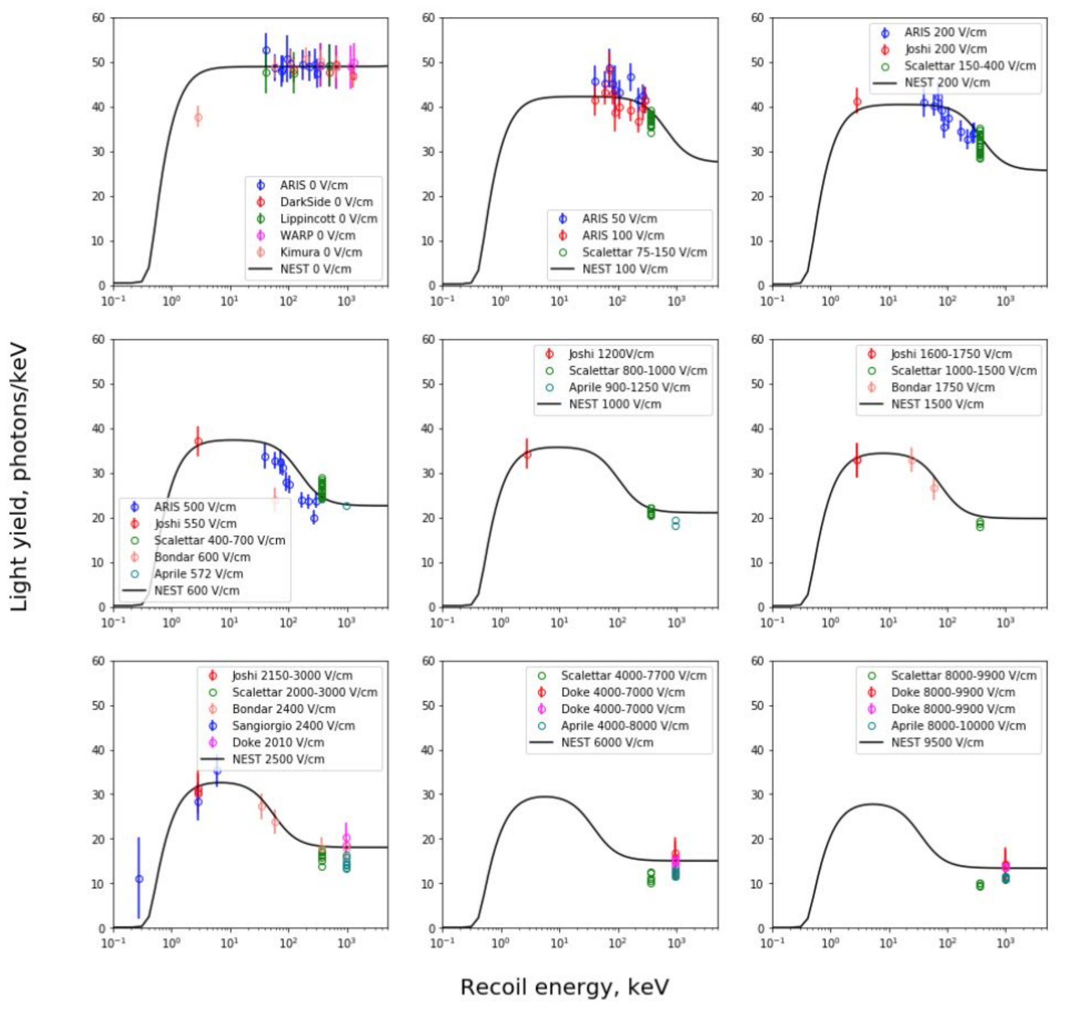
Backup



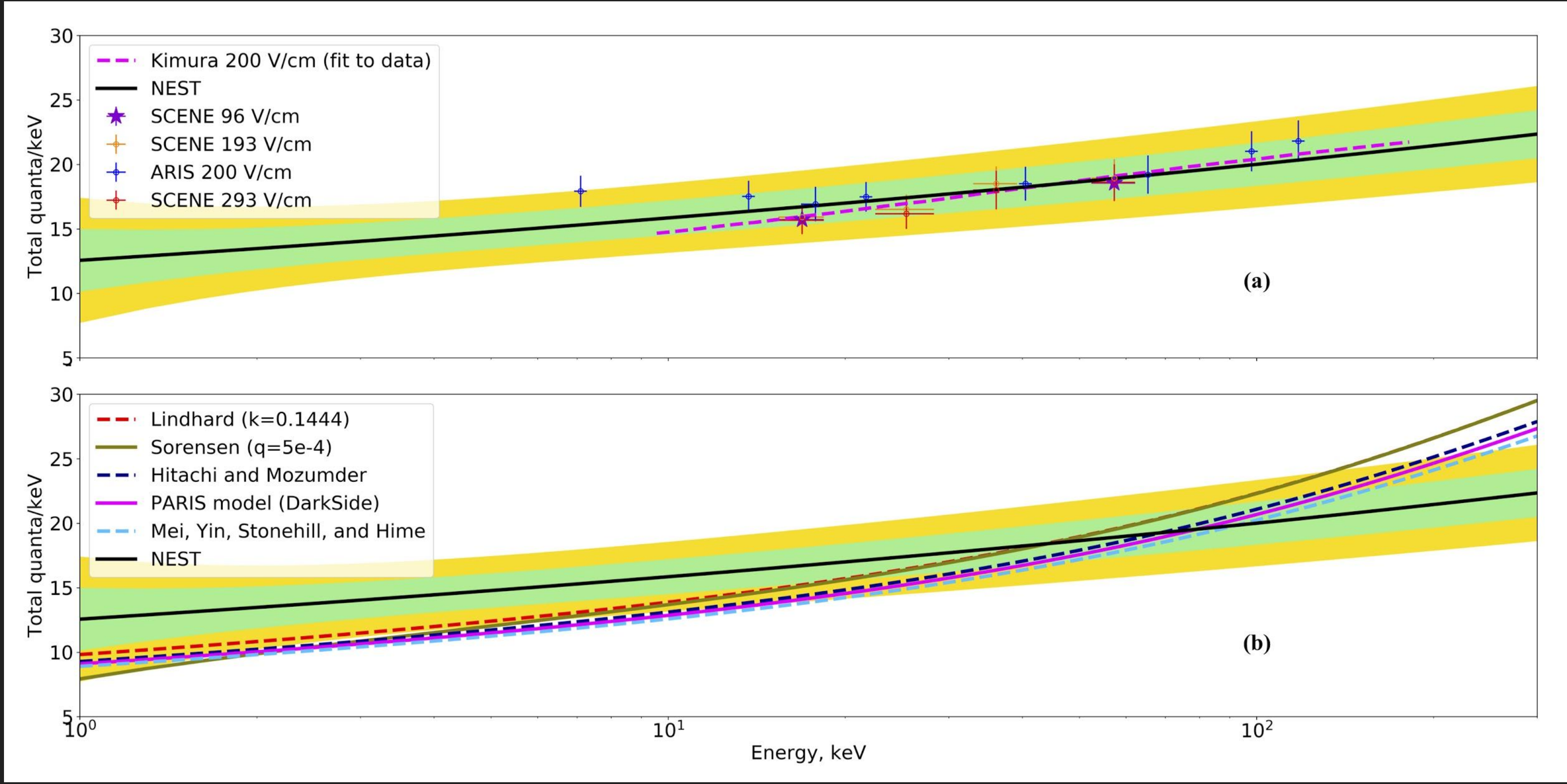
$N_{photons}$
1105 1381 1657 1934 2210
data
NEST
(a)
arbitrary
S1c [phe]
$N_{electrons}$
175 350 526 701 876
(b)
S2c [phe]
N_{quanta}
1868 1972 2076 2180 2284 2387 2491
(c)
arbitrary
E [keVee]
combined, NEST
(3% S1 noise, 0% S2 noise, uniform E-field)
data
(DS 2016)
200 V/cm
(d)
σ_E/μ_E [%]
E [keV]

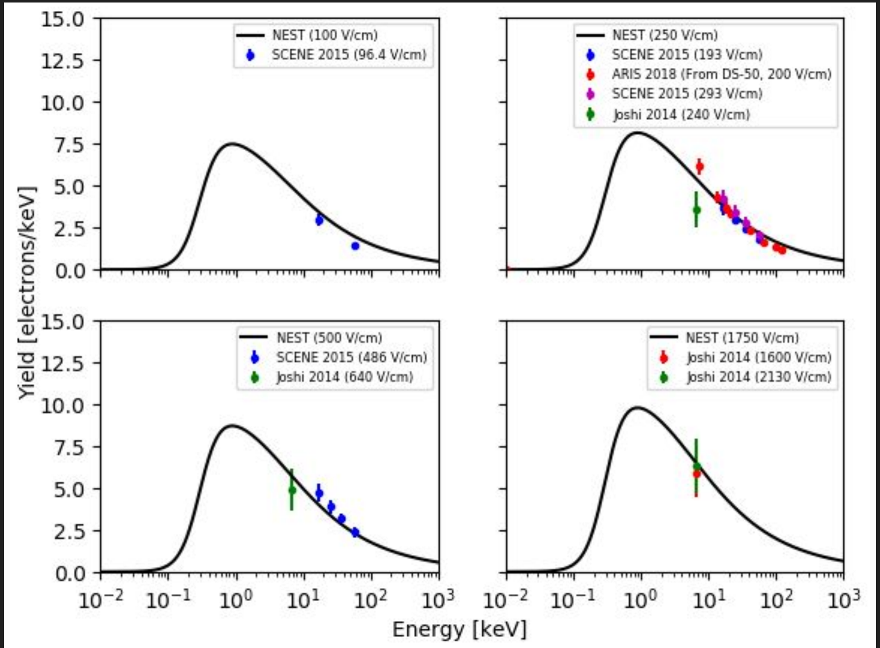


Ionization yield, electrons/keV
Recoil energy, keV
ARIS 0 V/cm
DarkSide 0 V/cm
Lippincott 0 V/cm
WARP 0 V/cm
Kimura 0 V/cm
Doke 0 V/cm
NEST 0 V/cm
ARIS 50 V/cm
ARIS 100 V/cm
Scalettar 75-150 V/cm
NEST 100 V/cm
ARIS 200 V/cm
Joshi 200 V/cm
Scalettar 150-400 V/cm
NEST 200 V/cm
ARIS 500 V/cm
Joshi 550 V/cm
Scalettar 400-700 V/cm
Bondar 600 V/cm
Aprile 572 V/cm
NEST 600 V/cm
Joshi 1200V/cm
Scalettar 800-1000 V/cm
Doke 1210 V/cm
Aprile 900-1250 V/cm
NEST 1000 V/cm
Joshi 1600-1750 V/cm
Scalettar 1000-1500 V/cm
Bondar 1750 V/cm
NEST 1500 V/cm
Joshi 2150-3000 V/cm
Scalettar 2000-3000 V/cm
Bondar 2400 V/cm
Sangiorgio 2400 V/cm
Doke 2010 V/cm
NEST 2500 V/cm
Scalettar 4000-7700 V/cm
Doke 4000-7000 V/cm
Doke 4000-7000 V/cm
Aprile 4000-8000 V/cm
NEST 6000 V/cm
Scalettar 8000-9900 V/cm
Doke 8000-9900 V/cm
Doke 8000-9900 V/cm
Aprile 8000-10000 V/cm
NEST 9500 V/cm

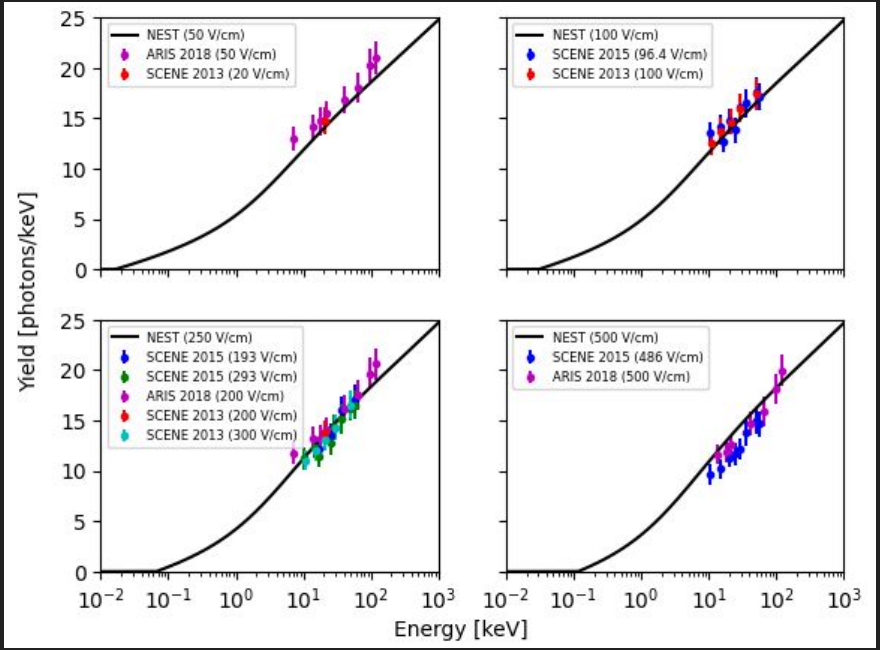


ARIS 0 V/cm
DarkSide 0 V/cm
Lippincott 0 V/cm
WARP 0 V/cm
Kimura 0 V/cm
NEST 0 V/cm
ARIS 50 V/cm
ARIS 100 V/cm
Scalettar 75-150 V/cm
NEST 100 V/cm
ARIS 200 V/cm
Joshi 200 V/cm
Scalettar 150-400 V/cm
NEST 200 V/cm
ARIS 500 V/cm
Joshi 550 V/cm
Scalettar 400-700 V/cm
Bondar 600 V/cm
Aprile 572 V/cm
NEST 600 V/cm
Joshi 1200V/cm
Scalettar 800-1000 V/cm
Aprile 900-1250 V/cm
NEST 1000 V/cm
Joshi 1600-1750 V/cm
Scalettar 1000-1500 V/cm
Bondar 1750 V/cm
NEST 1500 V/cm
Joshi 2150-3000 V/cm
Scalettar 2000-3000 V/cm
Bondar 2400 V/cm
Sangiorgio 2400 V/cm
Doke 2010 V/cm
NEST 2500 V/cm
Scalettar 4000-7700 V/cm
Doke 4000-7000 V/cm
Doke 4000-7000 V/cm
Aprile 4000-8000 V/cm
NEST 6000 V/cm
Scalettar 8000-9900 V/cm
Doke 8000-9900 V/cm
Doke 8000-9900 V/cm
Aprile 8000-10000 V/cm
NEST 9500 V/cm
Light yield, photons/keV
Recoil energy, keV


Kimura 200 V/cm (fit to data)
NEST
SCENE 96 V/cm
SCENE 193 V/cm
ARIS 200 V/cm
SCENE 293 V/cm
(a)
Lindhard (k=0.1444)
Sorensen (q=5e-4)
Hitachi and Mozumder
PARIS model (DarkSide)
Mei, Yin, Stonehill, and Hime
NEST
(b)
Total quanta/keV
Energy, keV



NEST (100 V/cm)
SCENE 2015 (96.4 V/cm)
NEST (250 V/cm)
SCENE 2015 (193 V/cm)
ARIS 2018 (From DS-50, 200 V/cm)
SCENE 2015 (293 V/cm)
Joshi 2014 (240 V/cm)
NEST (500 V/cm)
SCENE 2015 (486 V/cm)
Joshi 2014 (640 V/cm)
NEST (1750 V/cm)
Joshi 2014 (1600 V/cm)
Joshi 2014 (2130 V/cm)
Yield [electrons/keV]
Energy [keV]



NEST (50 V/cm)
ARIS 2018 (50 V/cm)
SCENE 2013 (20 V/cm)
NEST (100 V/cm)
SCENE 2015 (96.4 V/cm)
SCENE 2013 (100 V/cm)
NEST (250 V/cm)
SCENE 2015 (193 V/cm)
SCENE 2015 (293 V/cm)
ARIS 2018 (200 V/cm)
SCENE 2013 (200 V/cm)
SCENE 2013 (300 V/cm)
NEST (500 V/cm)
SCENE 2015 (486 V/cm)
ARIS 2018 (500 V/cm)
Yield [photons/keV]
Energy [keV]