Understanding Ionization, Scintillation Light, and the Energy Scale

In Noble Element Detectors

http://nest.physics.ucdavis.edu/site/

Matthew Szydagis, UC Davis

University of Connecticut 12/09/13

Why Noble Elements?

- Well suited to the **direct detection of dark matter** WIMPs (Weakly Interacting Massive Particles)
  - Xenon and argon both used, in both large dark matter experiments and small-scale calibration efforts
  - 1- and 2-phase, and zero and non-zero field (TPCs)
- Broad, compelling ν physics programs, like LBNE
  - Neutrinoless double-beta decay (^{136}Xe): EXO, NEXT
  - Coherent ν-scattering, and reactor monitoring: RED
- PET scans for medical applications (511 keV γ's)
- $\mu^- \Rightarrow e^- + \gamma$ (evidence of new physics): MEG, not to mention countless HEP detection applications

Direct WIMP Detection

- Body of evidence extensive for dark matter
  - Best-fit model for explaining the angular power spectrum of the CMB temperature anisotropy
  - Gravitational lensing
  - Large-scale structure observations and simulations
  - Galactic rotation curves
- All these point to a significant non-baryonic, non-relativistic component of matter (~85% of the matter or ~25% of total mass-energy in universe)
- WIMP is one possible candidate, and most searches are geared towards finding WIMPs
- Low-energy nuclear recoil (NR) are expected, and electron recoil (ER) constitute background

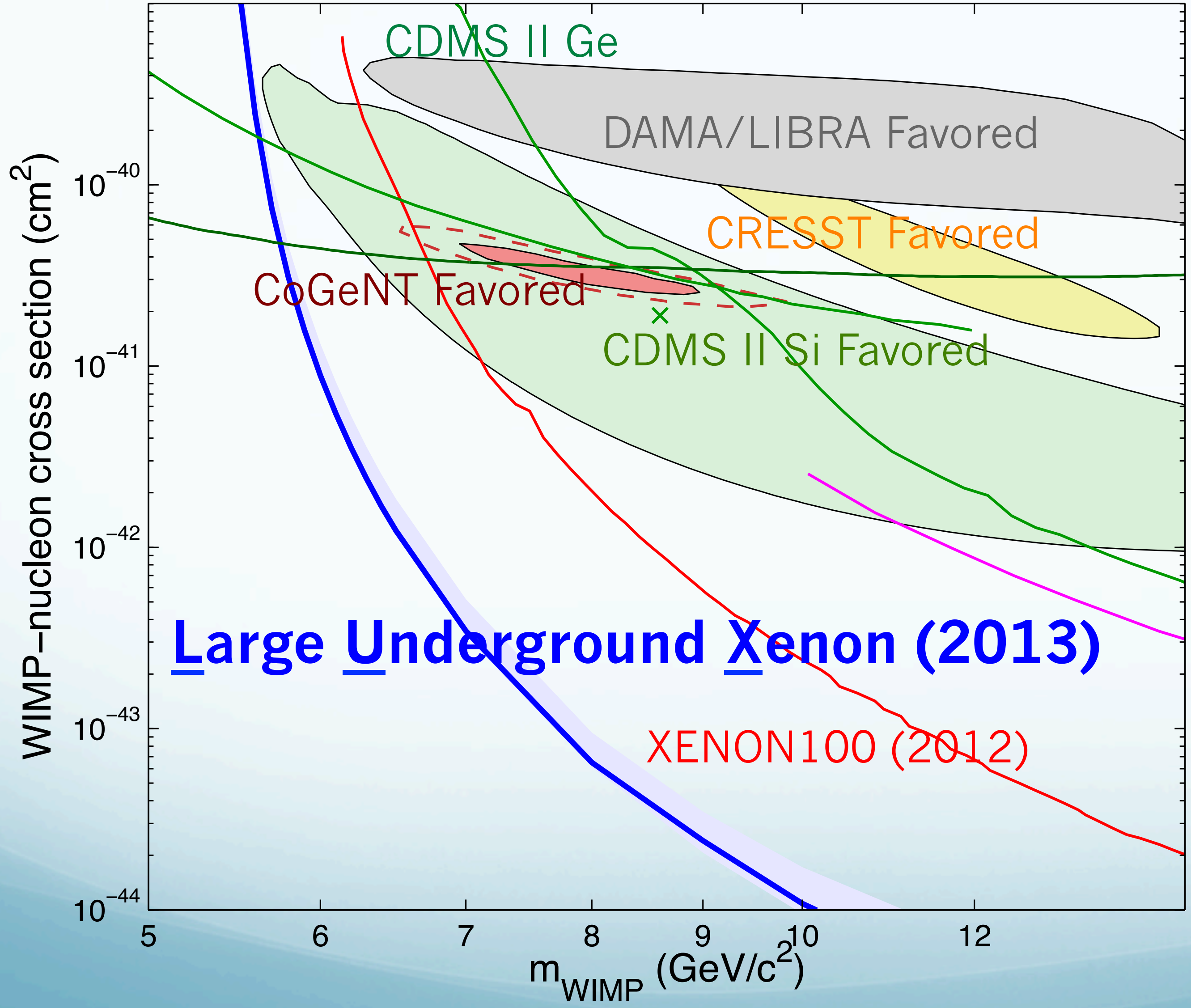
Gravitational Lensing Example

Image credit: Bell Labs

Galaxy Cluster Abell 2218 **HST • WFPC2**

NASA, A. Fruchter and the ERO Team (STScI) • STScI-PRC00-08

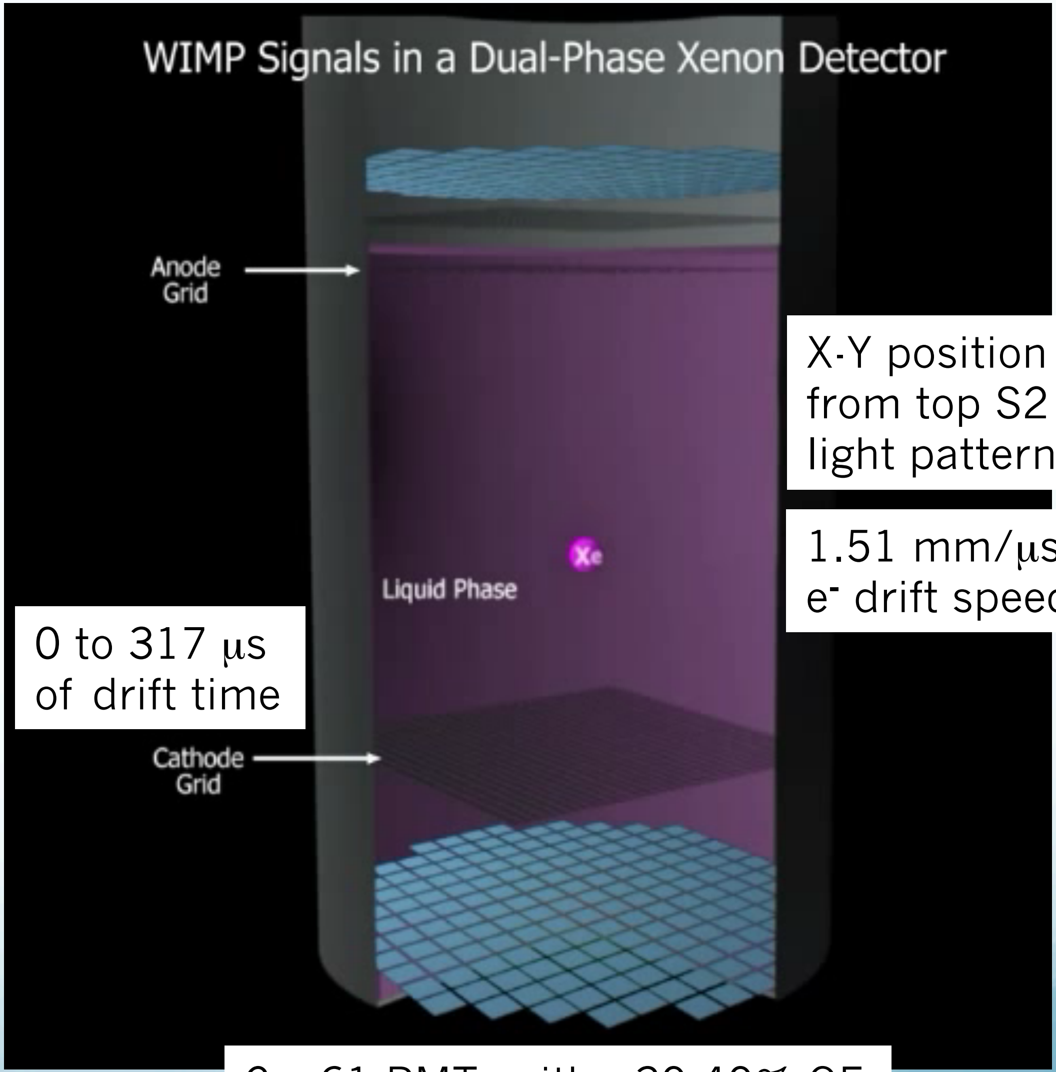
Why Understanding Matters



- Recent results (XENON and LUX collaborations) in conflict with low-mass WIMP interpretations of signals observed in CoGeNT, CDMS, and elsewhere
- Crucial to measure, model, and understand the detector response to NR in order to know for sure whether low-mass WIMPs ruled out or not by **xenon**

Two-Phase Technology

- Liquid + gas xenon time-projection chamber (TPC): LUX values as example
- Fiducialization and multiple-scattering rejection powerful: LXe dense, so it has good self-shielding
- The ratio of S2 to S1 forms the heart of the NR vs. ER discrimination of the backgrounds (high)



X-Y position from top S2 light pattern

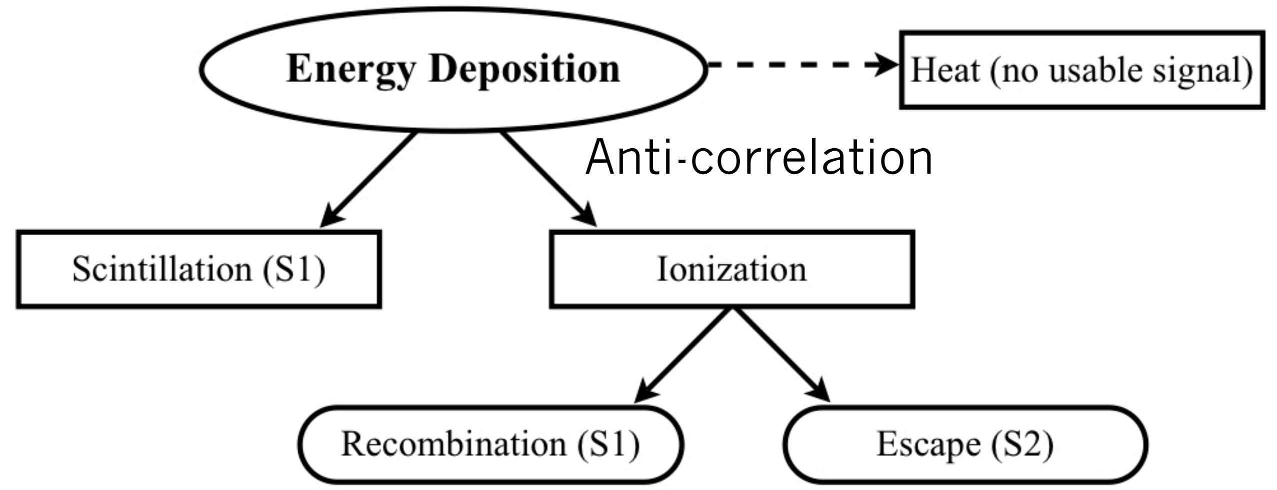
1.51 mm/μs e^- drift speed

0 to 317 μs of drift time

2 x 61 PMTs with ~30-40% QE

Physics of Nobles

- Energy ≠ S1: energy deposited into 3 channels ("heat" prominent for NR, reducing their S1 & S2)
- Excitation and recombination lead to the S1, while escaping ionization electrons lead to S2
- Scintillation comes from decaying molecules, not atoms. Not absorbed before it can be detected



Handled by NEST

- **N**oble **E**lement **S**imulation **T**echnique is a data-driven model explaining the scintillation and ionization yields of noble elements as a function of particle type, electric field, and *dE/dx* or energy

- Provides a full-fledged Monte Carlo (in Geant4) with
  - Mean yields: light AND charge, and photons/electron
  - Energy resolution: key in discriminating background
  - Pulse shapes: S1 AND S2, including single electrons

- The canon of existing experimental data was combed and all of the physics learned combined

M. Szydagis et al., JINST 8 (2013) C10003. arxiv:1307.6601
M. Szydagis et al., JINST 6 (2011) P10002. arxiv:1106.1613
J. Mock et al., Submitted to JINST (2013). arxiv:1310.1117

The Basic Principles

- The work function for creating an S1 photon or S2 electron does not depend on the interacting particle or its energy, but differences in yields are caused by the field, energy, and particle-dependent recombination probability of ionization electrons

- Recombination model is different for “short” tracks (< O(10) keV) and “long” tracks: using Thomas-Imel box (TIB) and Doke-Birks approaches, respectively

$$r = 1 - \frac{\ln(1+\xi)}{\xi}, \qquad \xi \equiv \frac{N_i \alpha'}{4a^2 v}$$

TIB model uses only total energy deposited, via number of ions

$$r = \frac{A\frac{dE}{dx}}{1 + B\frac{dE}{dx}} + C$$

By contrast, Doke-Birks relies on the energy loss

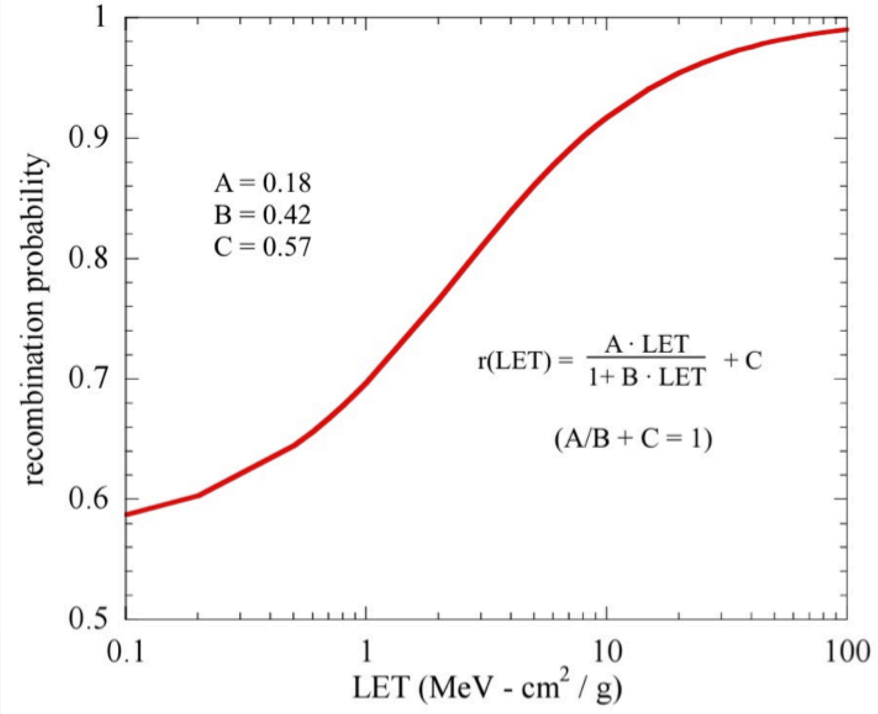
- This probability is what causes non-linear yields per unit of energy: twice the energy does not necessarily translate into twice the signal, in either channel

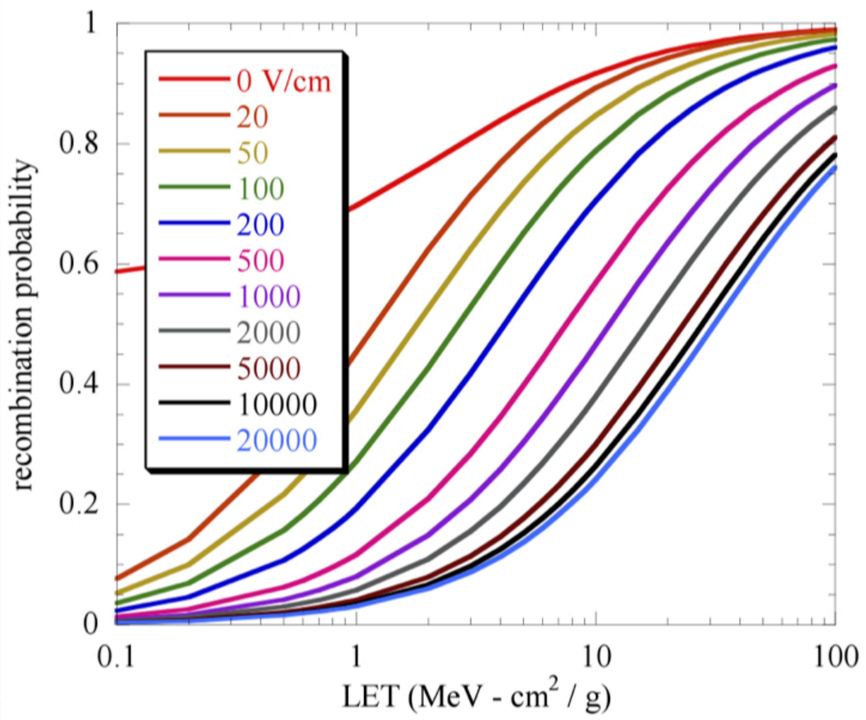
Life is Complicated

- Long-standings ways of thinking about signals from noble-element-based detectors shattered
  - In liquid Xe gamma-ray yields not flat in energy
  - Field dependence of yields also energy dependent
- Field dependence of light and charge yields for NR requires field or energy dependent exciton-ion ratio
- The NEST team dug up old, rare works, forgotten....

© 1991 Watterson (distributed by Universal Press Syndicate)

The Recombination Probability

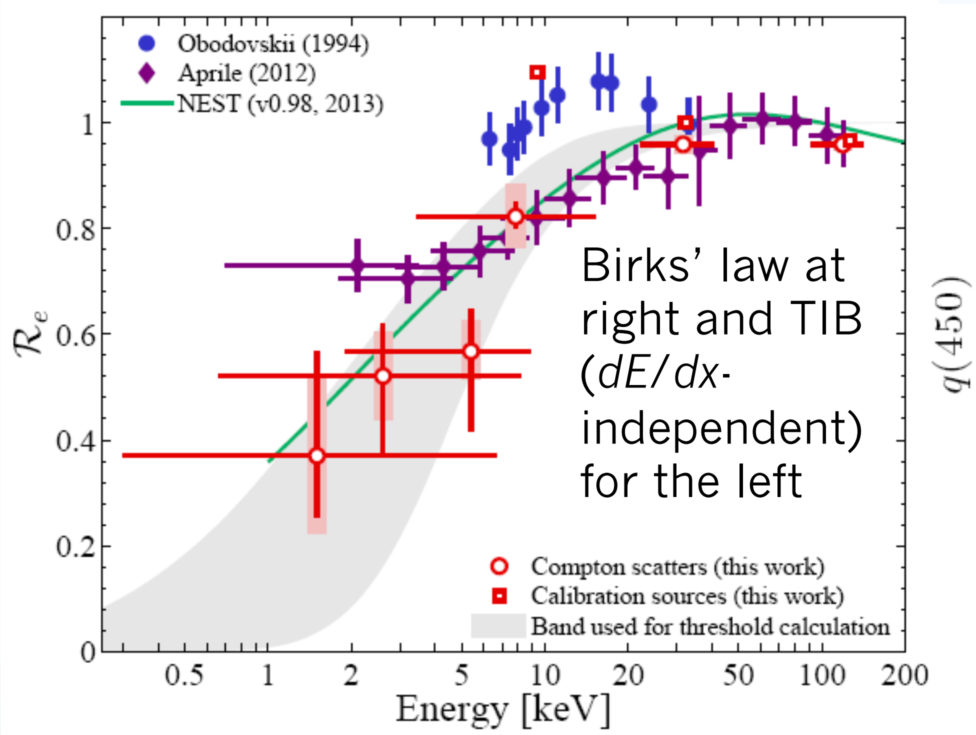




- A total number of quanta is generated for every *dE/dx* step in simulation
- Excitons and ions are separated binomially, and ions recombine, or not
- Function of *dE/dx* (Doke, above example) or N_i (TIB) with “constants” that vary with field, with Doke and TIB opposite in trend vs. total energy

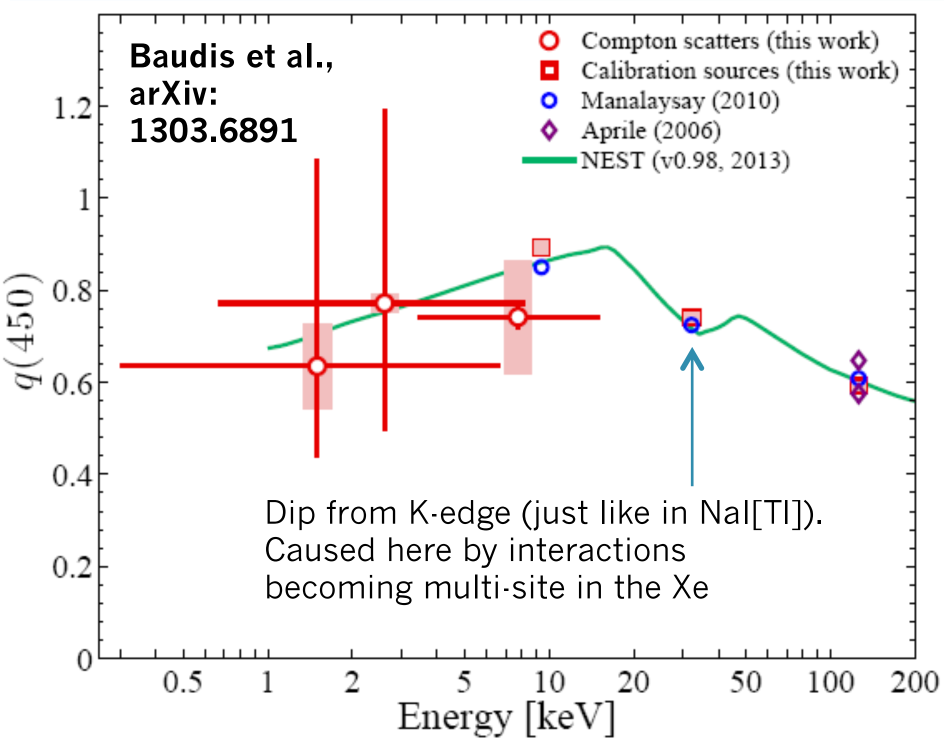
ER Scintillation Yield

Zero field



Birks' law at right and TIB (*dE/dx*-independent) for the left

Non-zero field (450 V/cm)

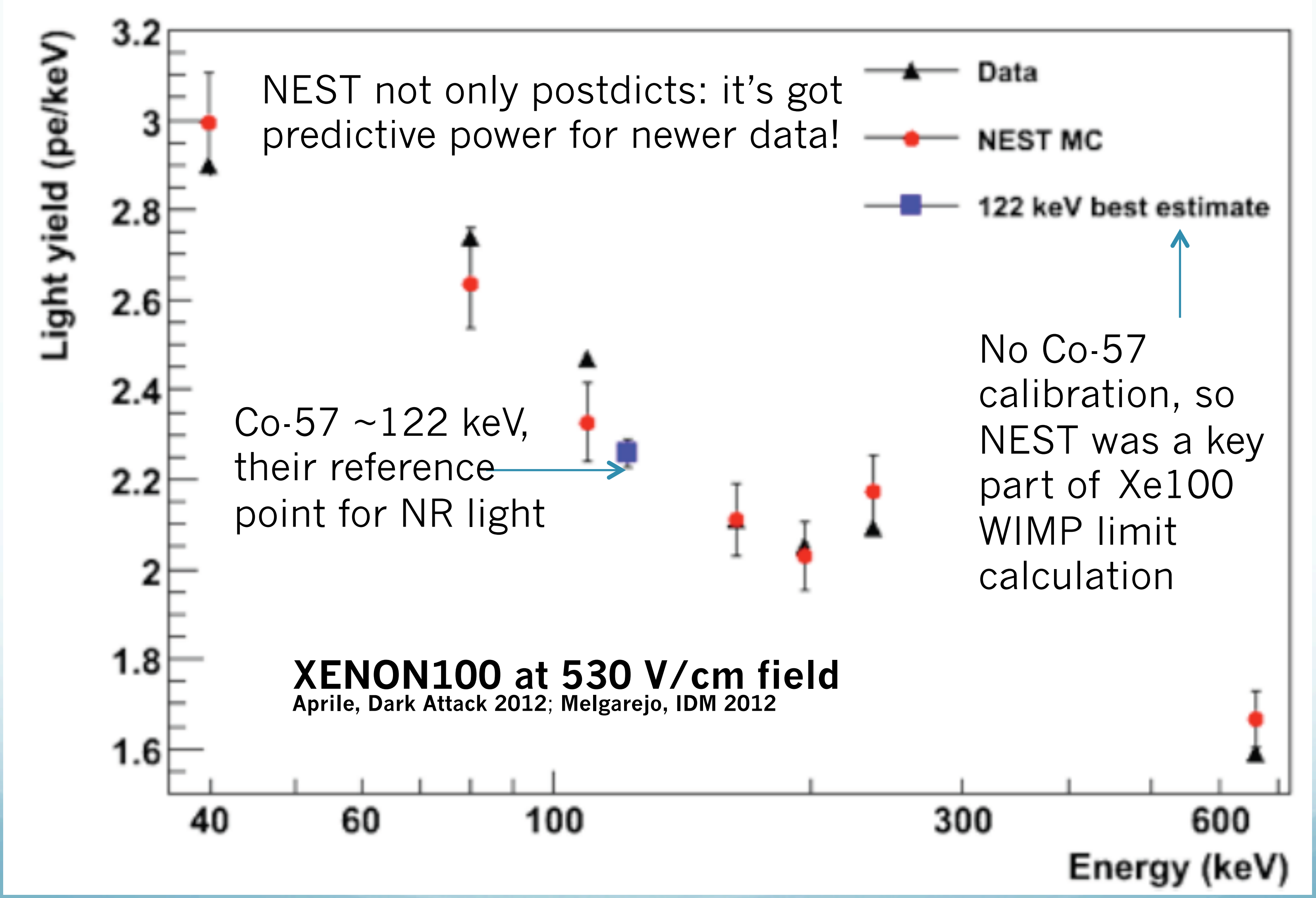


Baudis et al., arXiv: 1303.6891

Dip from K-edge (just like in NaI[Tl]). Caused here by interactions becoming multi-site in the Xe

- As the energy increases *dE/dx* decreases, thus recombination decreases: less light, at expense of more charge (Doke-Birks)
- At low energy (Thomas-Imel region) recombination increases with increasing energy, leading to more scintillation per keV

More Successful PREdictions

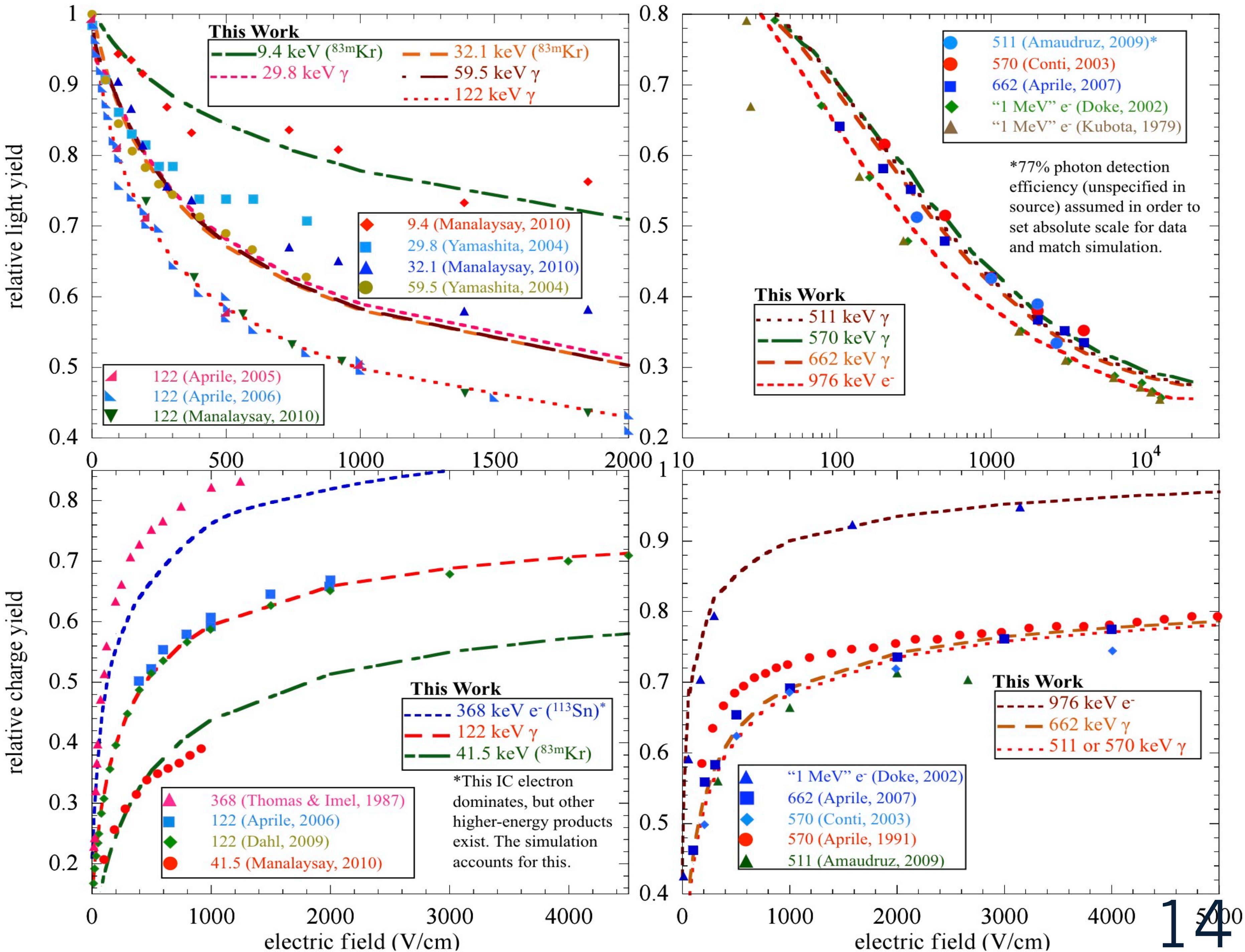


NEST not only postdicts: it's got predictive power for newer data!

Co-57 ~122 keV, their reference point for NR light

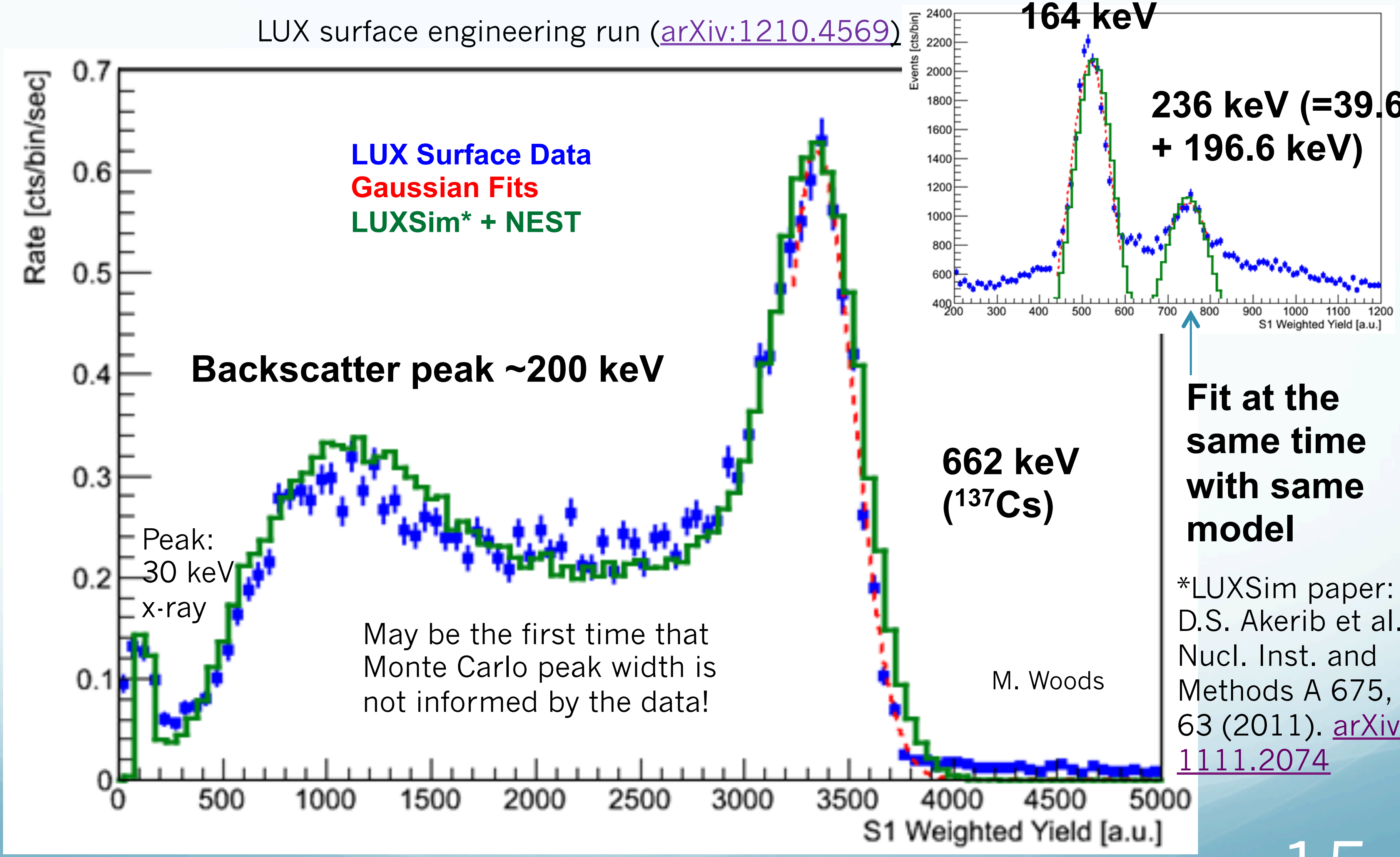
No Co-57 calibration, so NEST was a key part of Xe100 WIMP limit calculation

XENON100 at 530 V/cm field
Aprile, Dark Attack 2012; Melgarejo, IDM 2012


relative light yield
This Work
9.4 keV (^{83m}Kr)
32.1 keV (^{83m}Kr)
29.8 keV γ
59.5 keV γ
122 keV γ
9.4 (Manalaysay, 2010)
29.8 (Yamashita, 2004)
32.1 (Manalaysay, 2010)
59.5 (Yamashita, 2004)
122 (Aprile, 2005)
122 (Aprile, 2006)
122 (Manalaysay, 2010)
1
0.9
0.8
0.7
0.6
0.5
0.4
0
500
1000
1500
2000
0.8
0.7
0.6
0.5
0.4
0.3
0.2
10
100
1000
10^4
511 (Amaudruz, 2009)*
570 (Conti, 2003)
662 (Aprile, 2007)
"1 MeV" e$^-$ (Doke, 2002)
"1 MeV" e$^-$ (Kubota, 1979)
*77% photon detection efficiency (unspecified in source) assumed in order to set absolute scale for data and match simulation.
This Work
511 keV γ
570 keV γ
662 keV γ
976 keV e$^-$
relative charge yield
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0
1000
2000
3000
4000
electric field (V/cm)
This Work
368 keV e$^-$ (^{113}Sn)*
122 keV γ
41.5 keV (^{83m}Kr)
*This IC electron dominates, but other higher-energy products exist. The simulation accounts for this.
368 (Thomas & Imel, 1987)
122 (Aprile, 2006)
122 (Dahl, 2009)
41.5 (Manalaysay, 2010)
1
0.9
0.8
0.7
0.6
0.5
0.4
0
1000
2000
3000
4000
5000
electric field (V/cm)
This Work
976 keV e$^-$
662 keV γ
511 or 570 keV γ
"1 MeV" e$^-$ (Doke, 2002)
662 (Aprile, 2007)
570 (Conti, 2003)
570 (Aprile, 1991)
511 (Amaudruz, 2009)

Energy Resolution: LUX

LUX surface engineering run (arXiv:1210.4569)



Backscatter peak ~200 keV

Peak:
30 keV
x-ray

May be the first time that Monte Carlo peak width is not informed by the data!

662 keV (^{137}Cs)

M. Woods

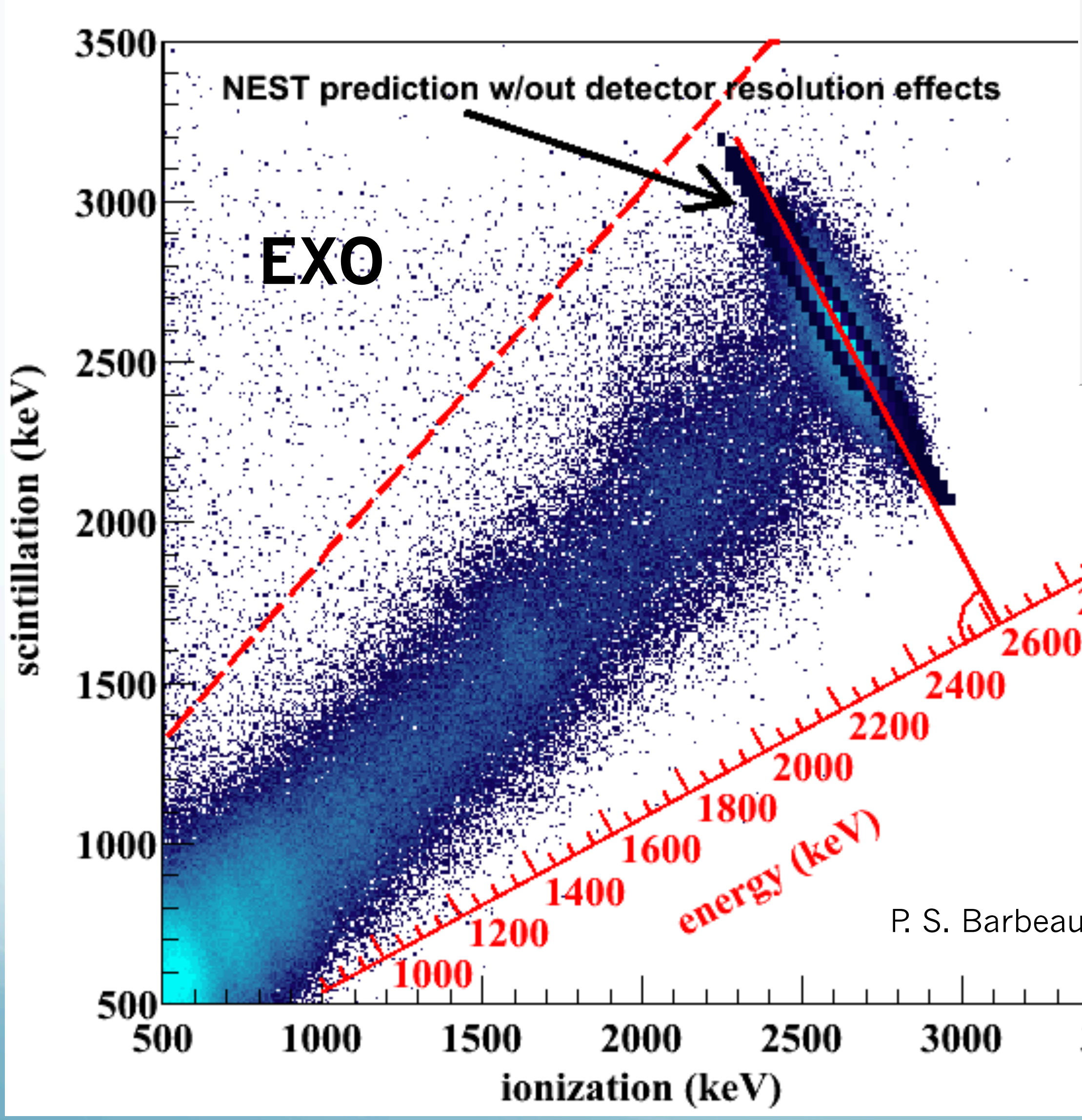
164 keV

236 keV (=39.6 + 196.6 keV)

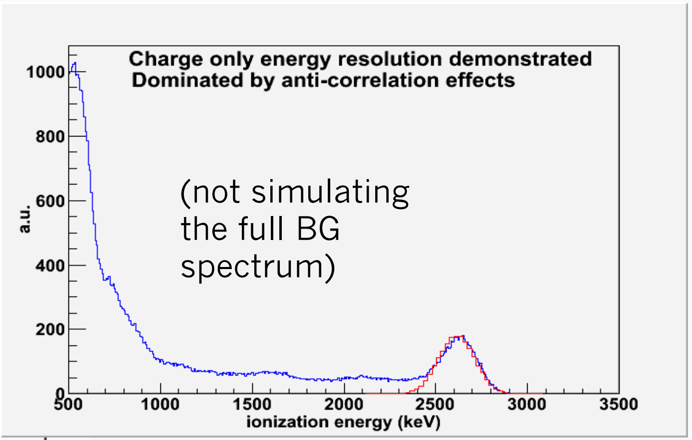
Fit at the same time with same model

*LUXSim paper: D.S. Akerib et al., Nucl. Inst. and Methods A 675, 63 (2011). arXiv:1111.2074

Energy Resolution: EXO



P. S. Barbeau



(not simulating the full BG spectrum)

- Prediction for a field never studied before (376 V/cm) and a new energy (2.6 MeV gammas, whereas NEST vetted at 0.57)
- The recombination fluctuations modeled as worse than binomial with a field-dependent Fano-like factor (big)

NEST-Based Energy Scale

~~$E_{\mathrm{nr}} = (S1/L_y)(1/\mathcal{L}_{\mathrm{eff}})(S_{\mathrm{ee}}/S_{\mathrm{nr}})$~~

$$E_{nr} = \mathcal{L}^{-1} \cdot (n_e + n_\gamma) \cdot W.$$

W_{LXe} = 13.7 +/- 0.2 eV

- Energy a linear combination of the number of primary photons n_γ and electrons n_e generated
- Photon count equal to S1 phe (XYZ-corrected with calibration events) divided by detection efficiency (light collection x PMT QE), and electron count is S2 phe (XYZ-corrected) divided by the product of extraction efficiency and the number of phe per e^-
- Scale calibrated using ER ($\mathcal{L}$=1). Hitachi-corrected* Lindhard factor assumed for NR (k=0.11 not 0.166)
- Matches LUX data, and others' measurements

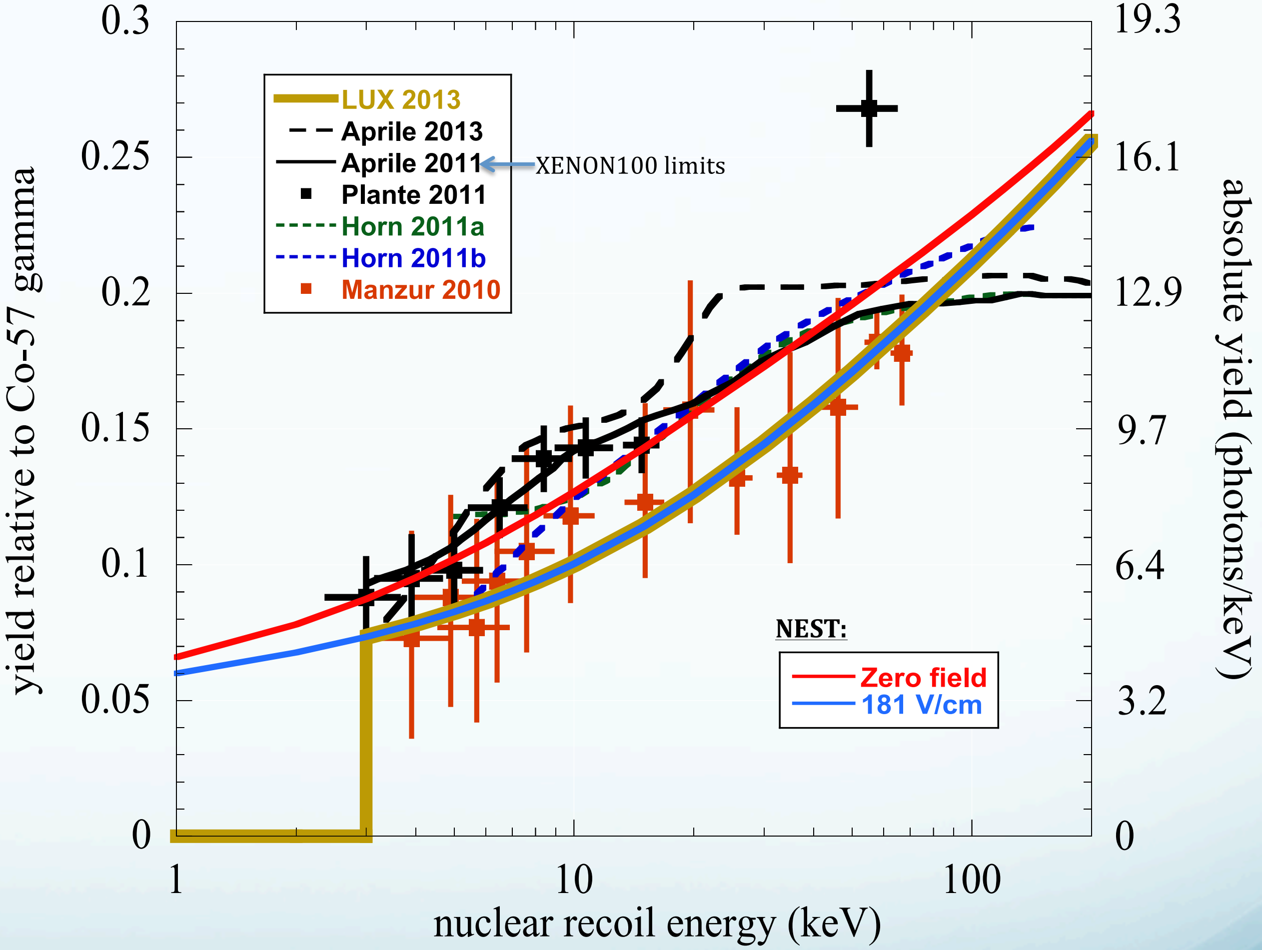
$$\mathcal{L} = \frac{kg(\epsilon)}{1 + kg(\epsilon)},$$

$$\epsilon = 11.5\,(E_{nr}/keV)\,Z^{(-7/3)},$$
$$g(\epsilon) = 3\epsilon^{0.15} + 0.7\epsilon^{0.6} + \epsilon,$$

* P. Sorensen and C. E. Dahl, Phys. Rev D 83 (2011) 063501, [arXiv: 1101.6080]

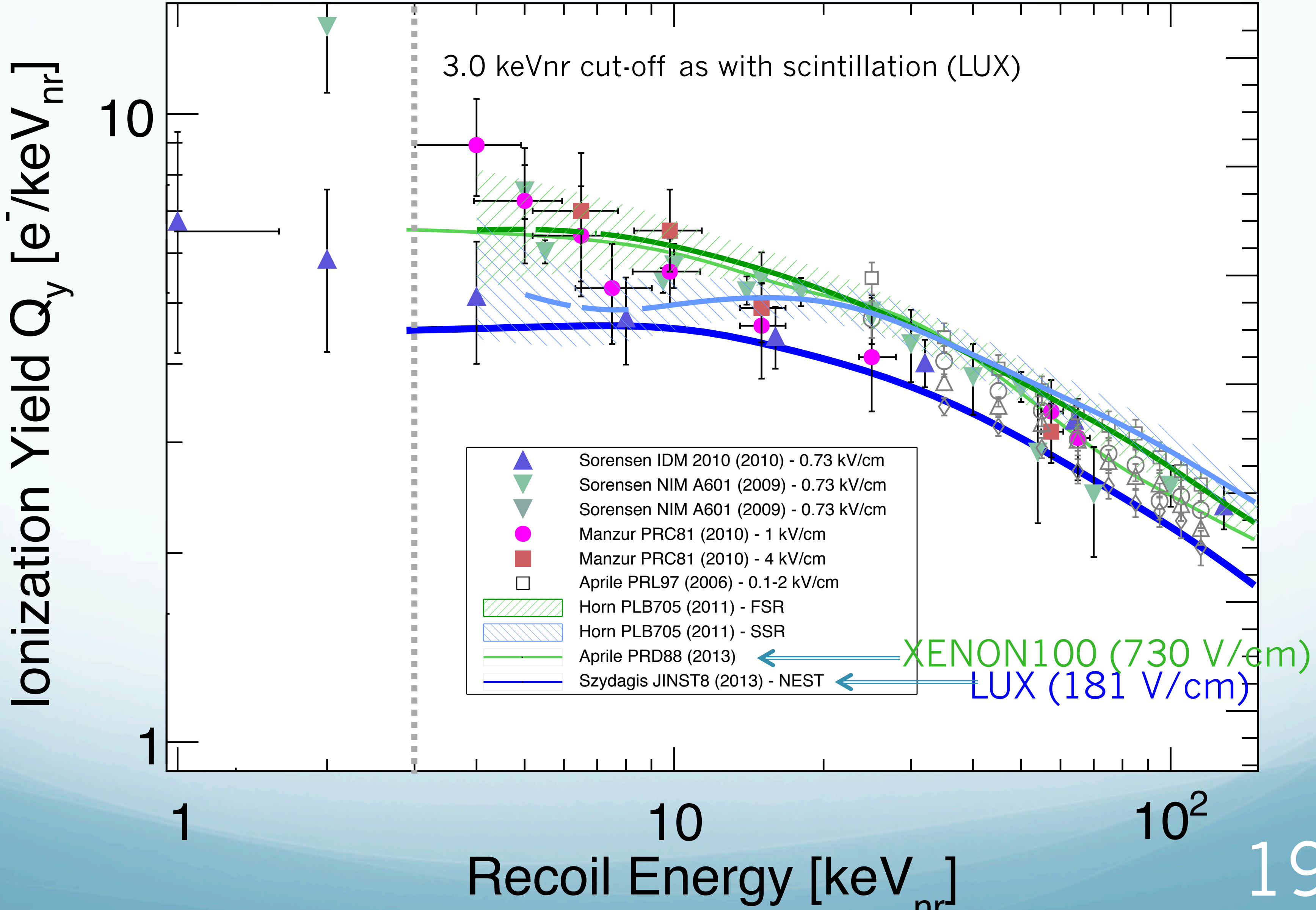
NR Scintillation Yield

- NEST uses thesis data (C.E. Dahl) from five different fields (60, 522, 876, 1951, 4060 V/cm), making NEST predictive for any electric field
  - Extracted energy-dependent light suppression factors (S_{nr}, S_{ee}) for electric field (at expense of charge via recombination probability)
  - Result is conservative approach (~0.8 of light at 181 V/cm compared to 0): compare with past (0.9-0.95 assumed, for higher fields) and liquid argon
- No need to use light yield of 63 photons/keV, Co-57 zero-field (can't penetrate anyway), and non-linearity in ER yield re-proven by recent Compton scattering data handled within NEST

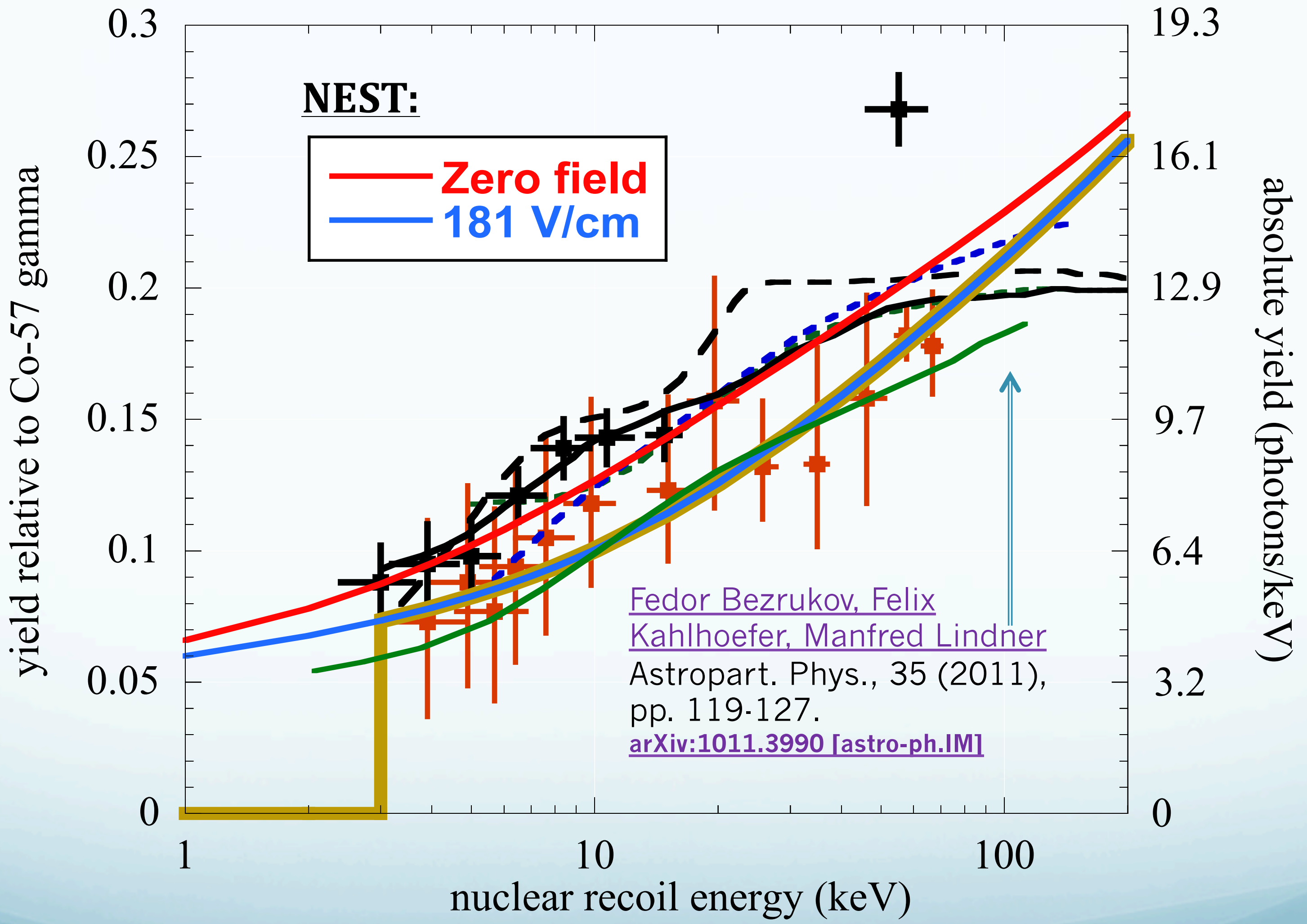


Data taken at non-zero field is translated by those reporting these results, assuming reduction of 0.95 (Aprile 2013, 730 V/cm) or 0.9 (Horn 2011, ~4000 V/cm, from ZEPLIN-III). LUX is 181 V/cm. All other data points actually taken at zero field. Note: NEST not a fit

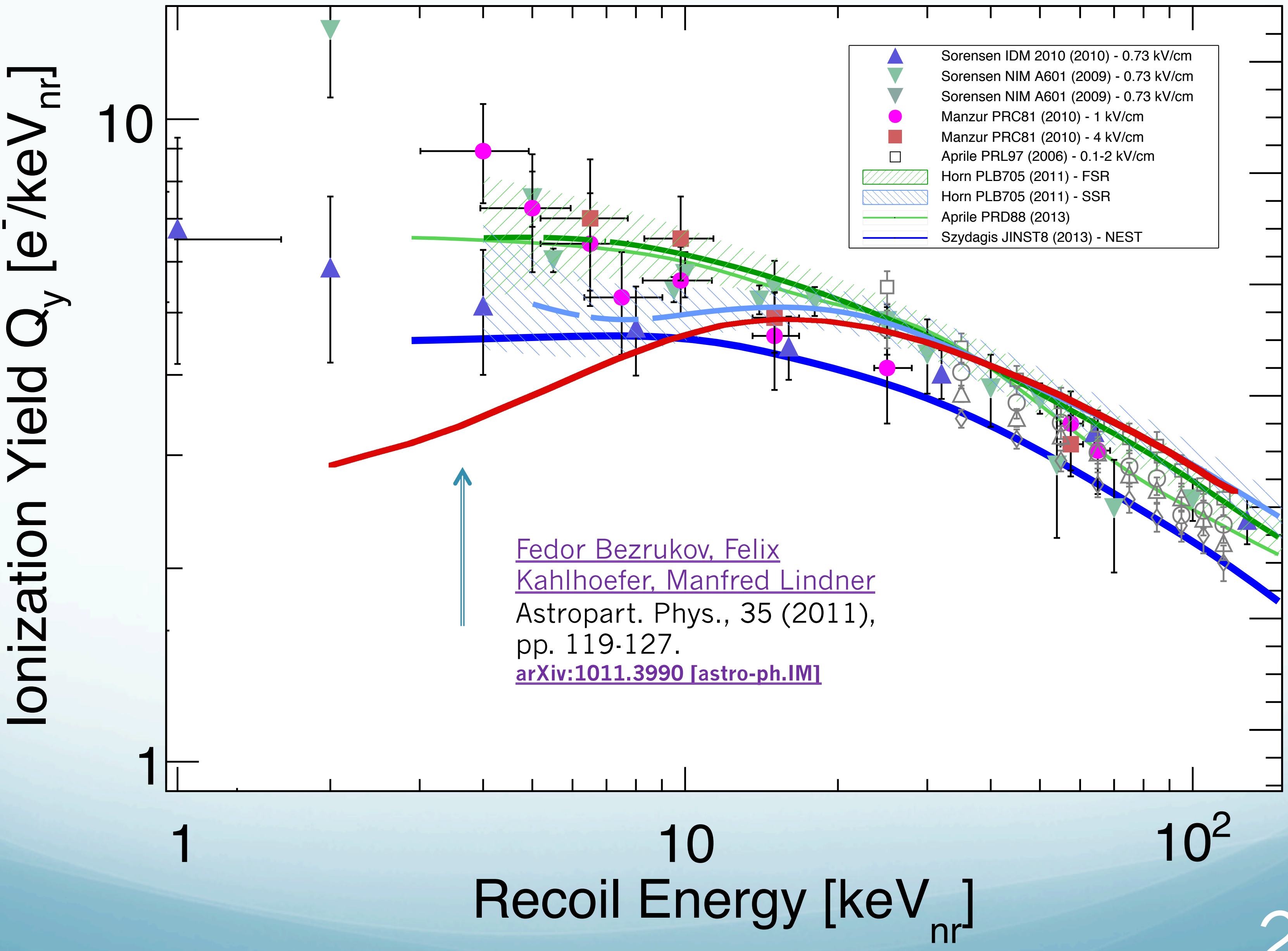
NR Ionization Yield



Pessimistic Case Comparison

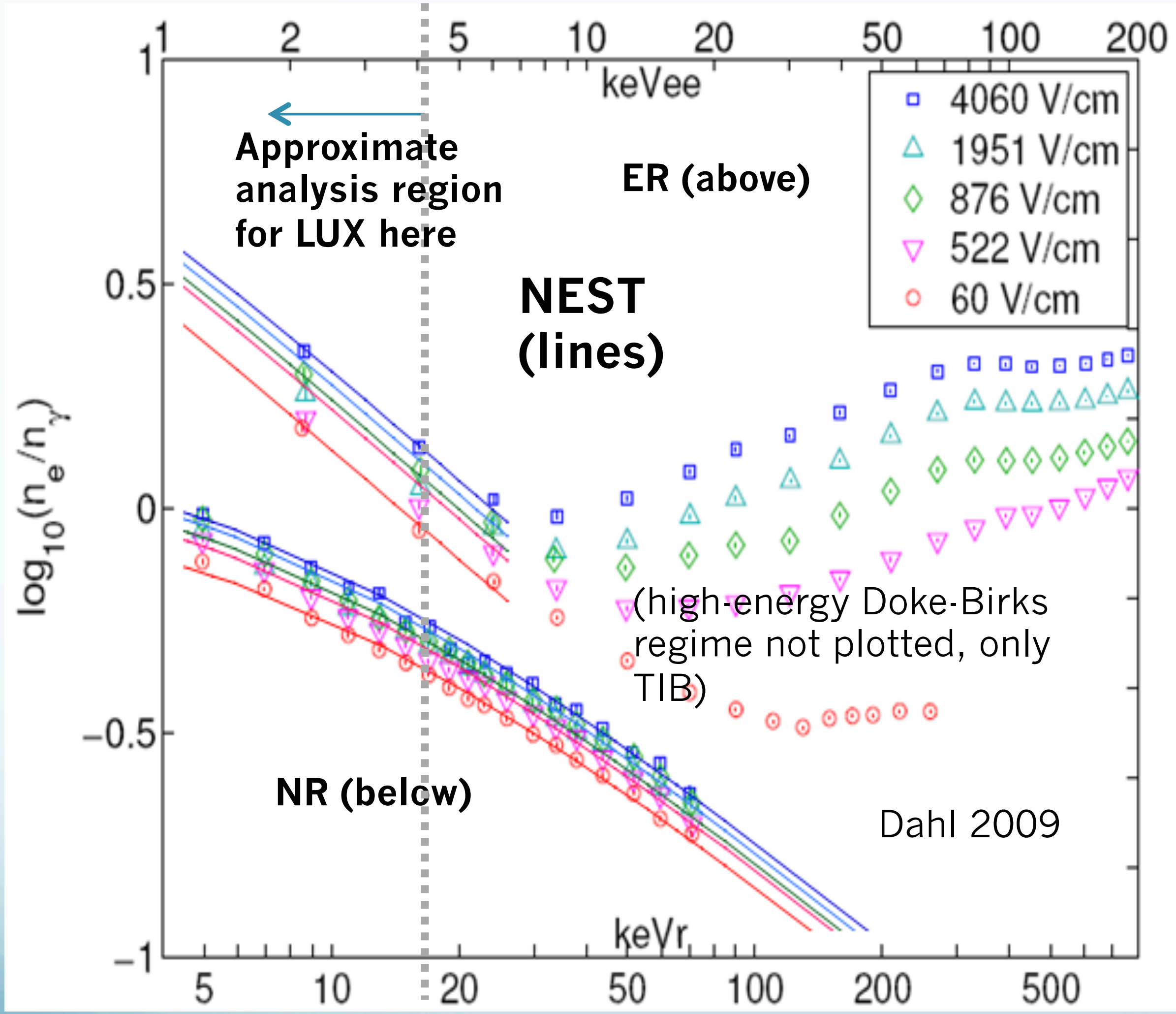


Fedor Bezrukov, Felix Kahlhoefer, Manfred Lindner
Astropart. Phys., 35 (2011), pp. 119-127.
arXiv:1011.3990 [astro-ph.IM]



Fedor Bezrukov, Felix Kahlhoefer, Manfred Lindner
Astropart. Phys., 35 (2011), pp. 119-127.
arXiv:1011.3990 [astro-ph.IM]

NR, ER “Bands”



Approximate analysis region for LUX here

ER (above)

NEST (lines)

(high-energy Doke-Birks regime not plotted, only TIB)

NR (below)

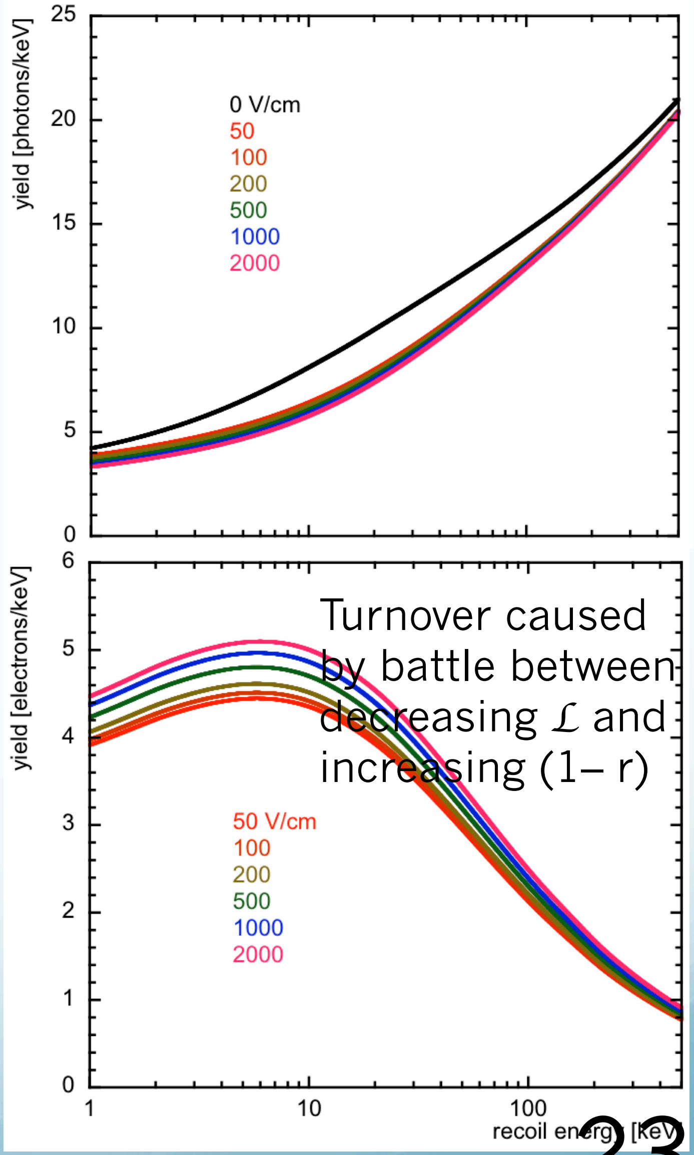
Dahl 2009

The keVnr energy scale shown here is Dahl’s, and assumes an old, flat $\mathcal{L} = 0.25$: using Hitachi, the 5 keVnr point is actually 8.67 and the 70 keVnr point is 85.5 (and this correction has been accounted for in NEST when fitting the data). The keVee scale is still correct.

- Data presented in terms of log(n_e/n_γ), converted from log(S2/S1), but keVee scale is (n_e+n_γ)*13.7e-3 keV and so can easily extract n_γ and n_e alone and get their field dependencies
- AmBe and Cf-252 sources, not an angle-tagged neutron scattering measurement, but important thing is *relative* yield is well-established

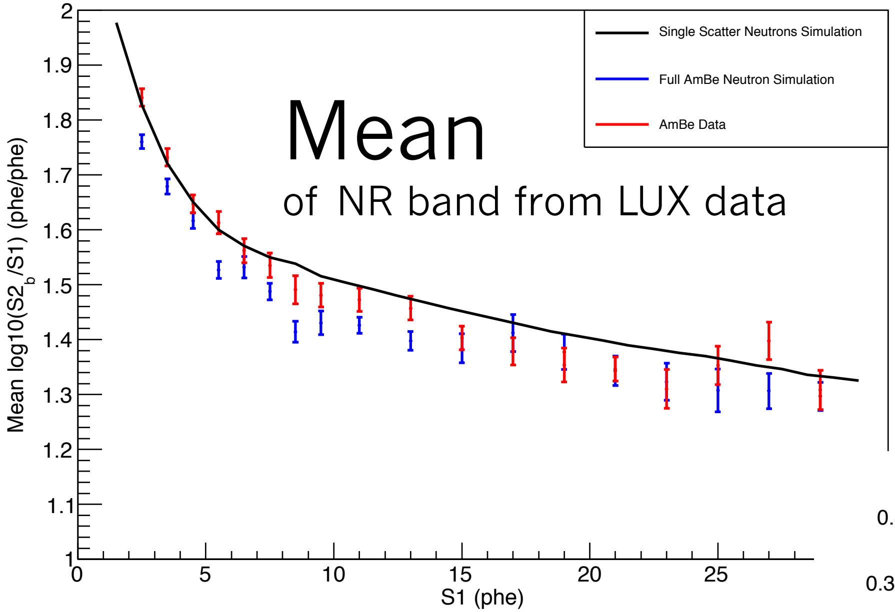
Electric Field Dependence

- Steep drop-off from zero to non-zero field (then slow change again) needed to simultaneously explain both Dahl thesis data AND zero field too, assuming same $\mathcal{L}$-factor
  - OR, Manzur not Plante at 0
- NEST is conservative, but more importantly, self-consistent
- Post-dictions based on fits to Dahl, so agreement with Manzur a pleasant accident
- Curves are straight-jacketed: quanta sum fixed by Hitachi *dE/dx* model, while Dahl gives us the ratio of charge to light

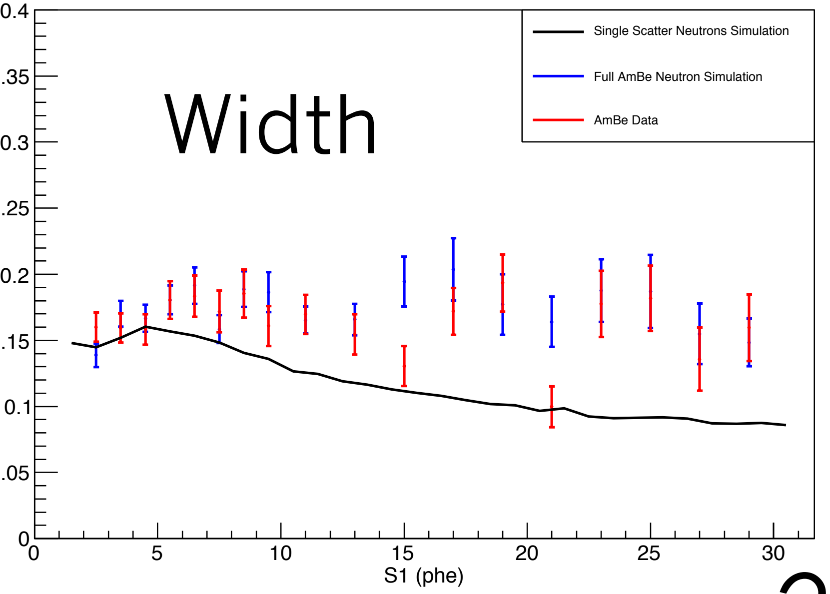


Turnover caused by battle between decreasing $\mathcal{L}$ and increasing (1– r)

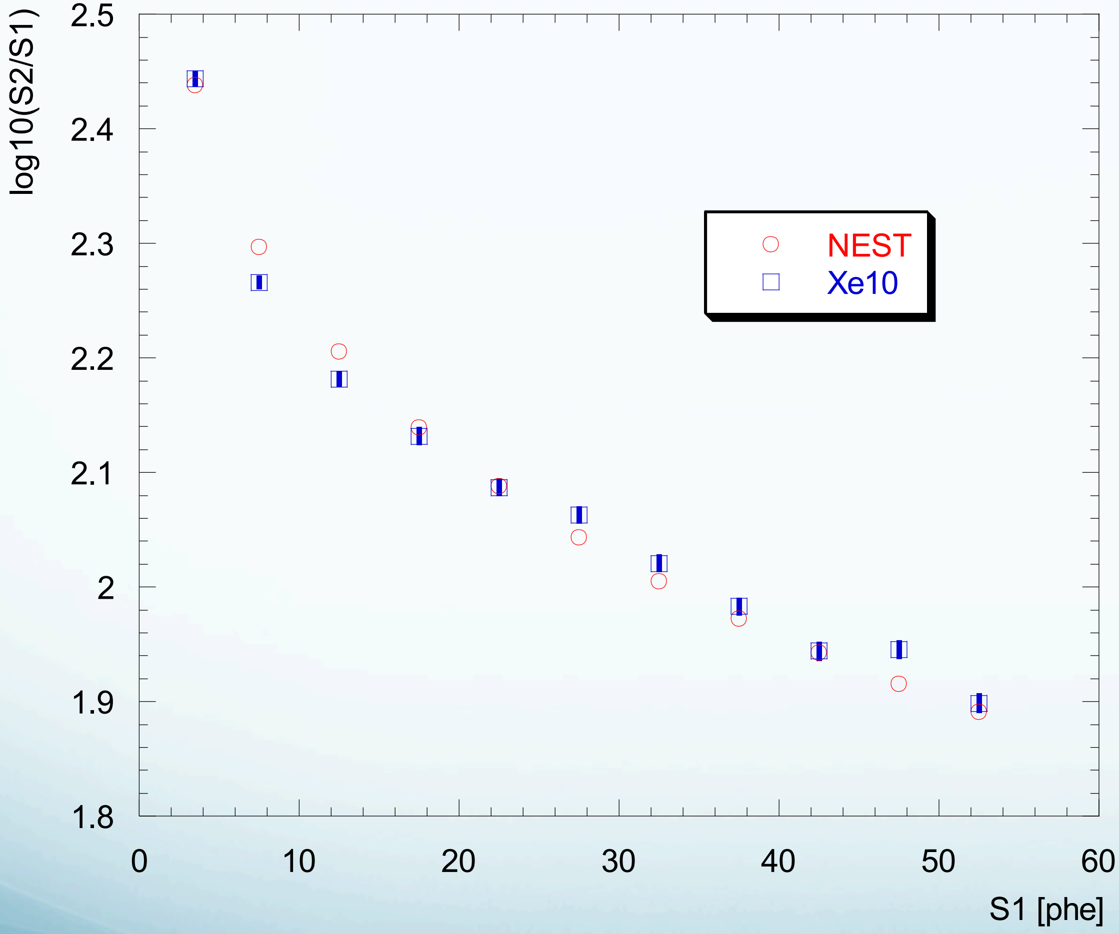
Back to Band



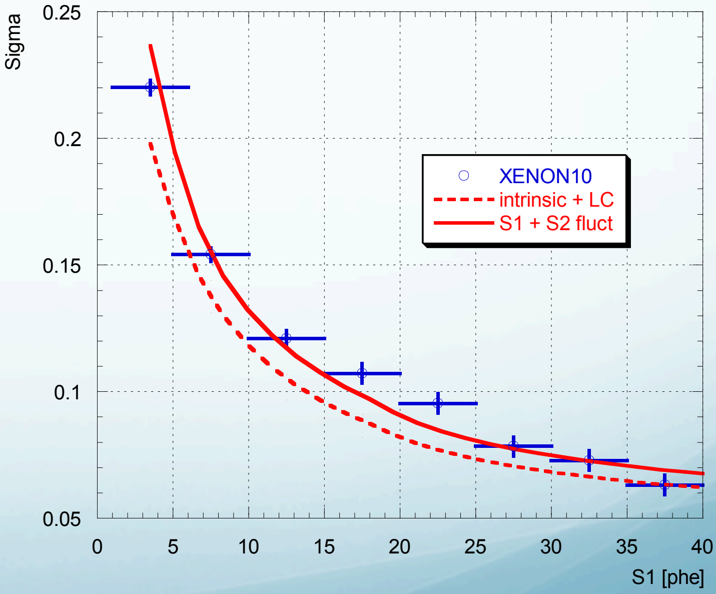
- Both single-scatter (WIMP-like) and full AmBe simulations use NEST, but AmBe sim includes ER component (Compton scatters) + neutron-X event (multiple-scatter, single-ionization) contamination
- Neutron-only effects shifting band mean and width in well-understood fashion, inapplicable to WIMP scattering. When they're included, there's agreement with data



Agreement with Past



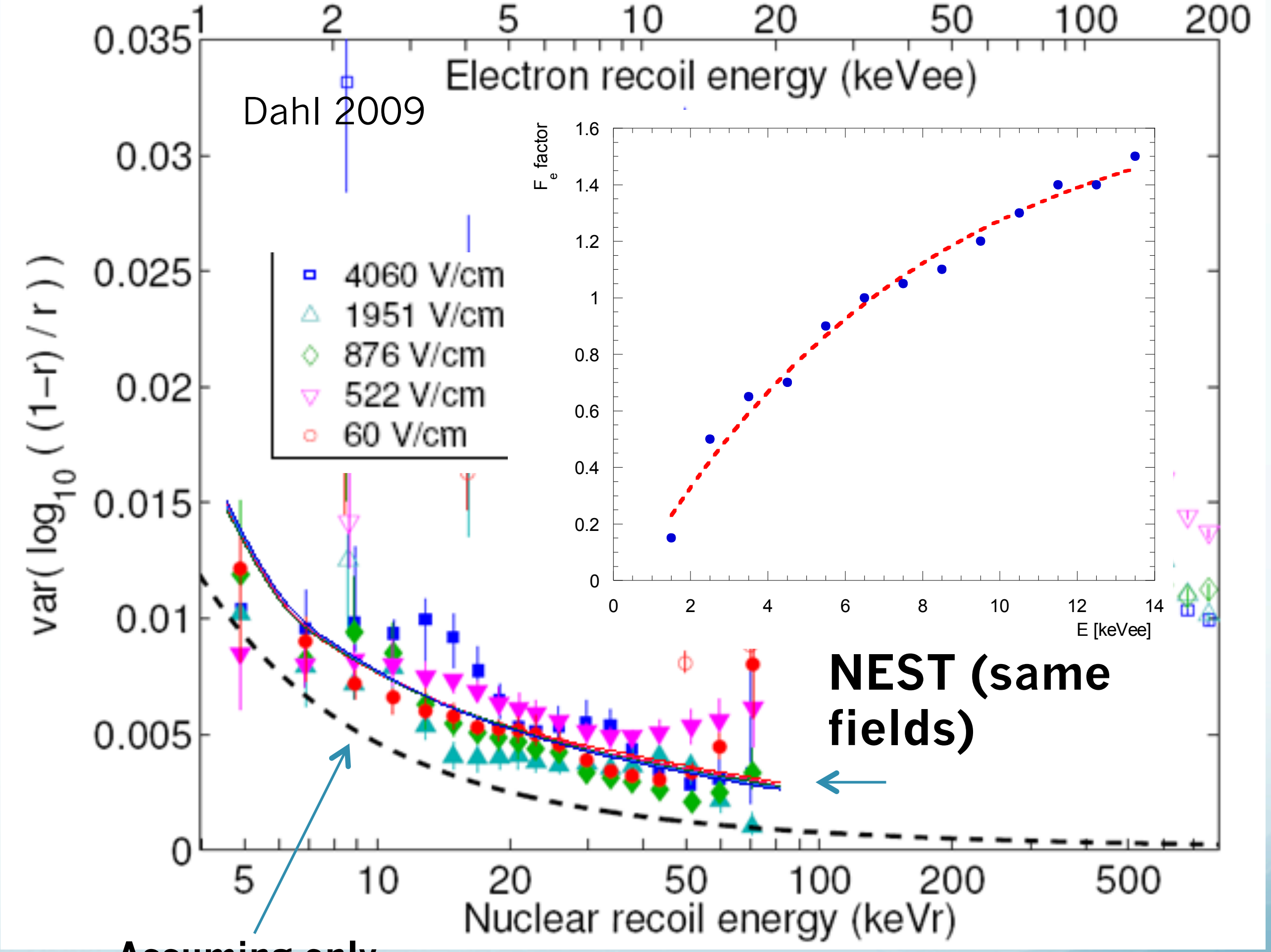
Band width and band mean for NR post-dicted for the old XENON10 data, after model construction based on Dahl, whose data are extensive in both field and energy, and who was the first to use a combined energy scale at low energies. In addition, he estimated intrinsic energy resolution, subtracting out the detector effects



Band Width Model

- Number of e⁻'s was varied as √ (F_e n_e) per interaction site
- Averaged over field (negligible evidence of electric field dependence) and found an increasing ionization Fano-like factor describes the data well (just like it does in case of ER)
- Rejected options of vanilla Fano and $\mathcal{L}$ factor fluctuations because no effect on band width seen

Ignore hollow (ER) points. NR is solid



Dahl 2009

NEST (same fields)

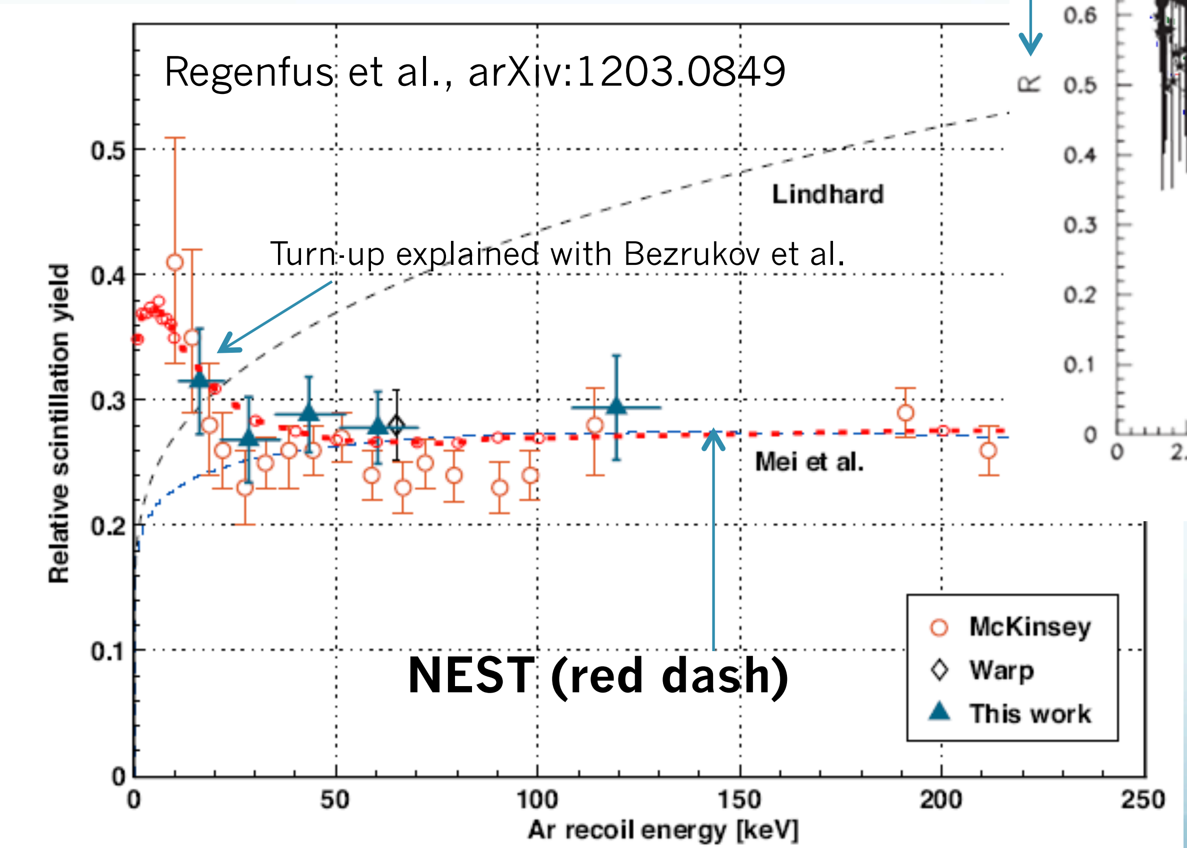
Assuming only binomial fluctuations

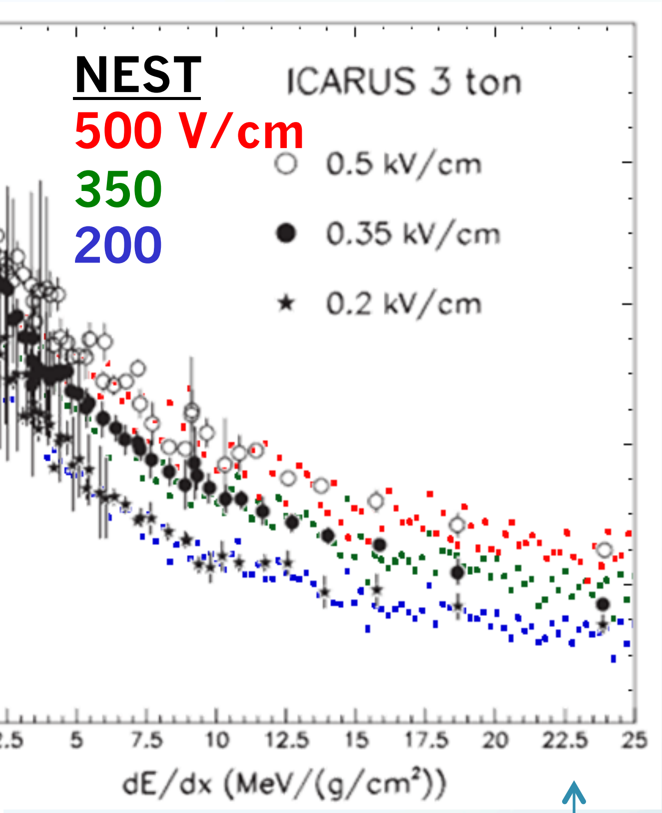
Y-axis is an analogue for the log10(S2/S1) width

Teaser for Argon

- Scintillation yield relative to ER is higher in Ar than in Xe
- Evidence of possible Ar-Ar cross-section enhancement

R=1–r is a way of checking both light and charge yields, concurrently

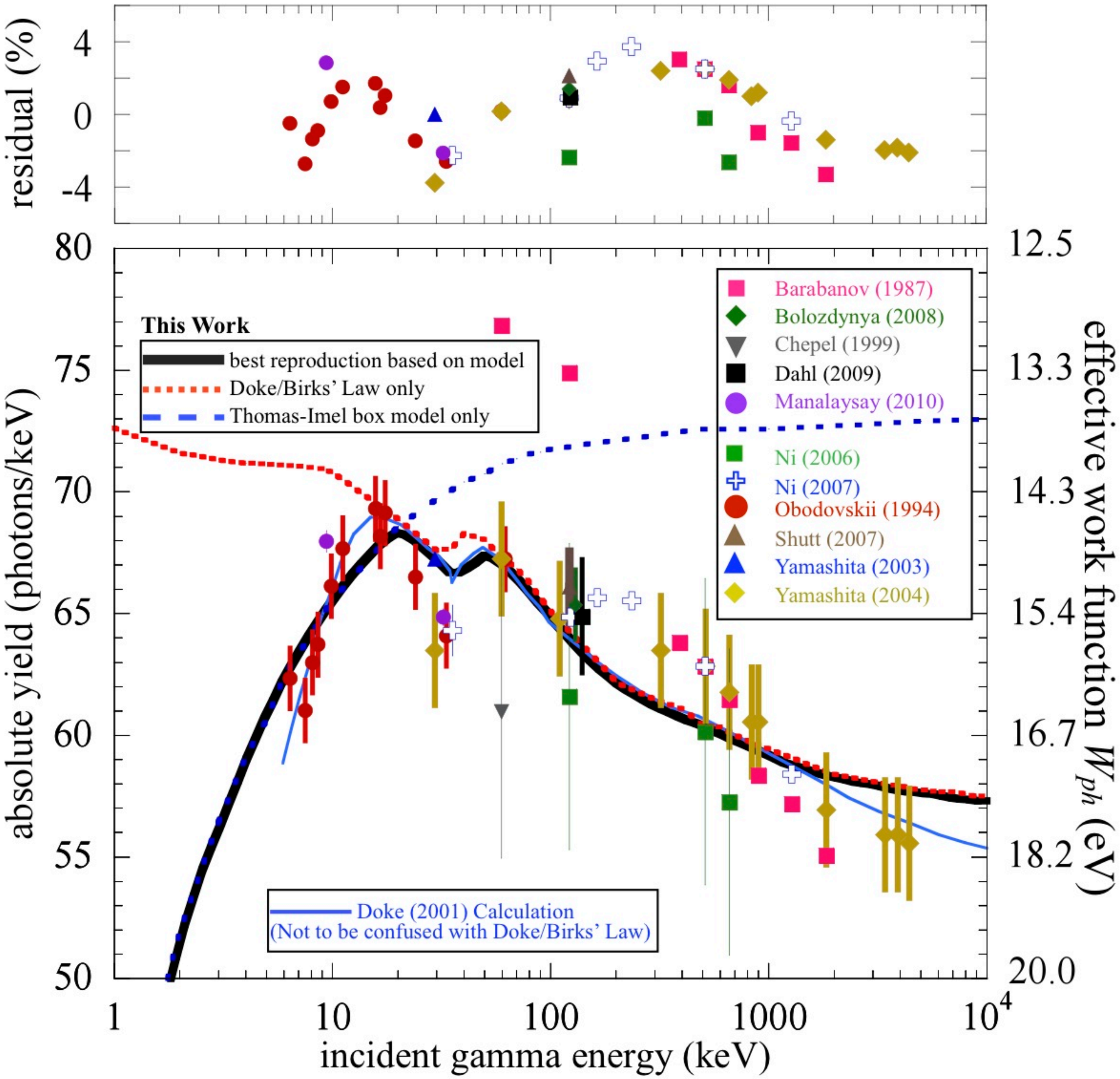


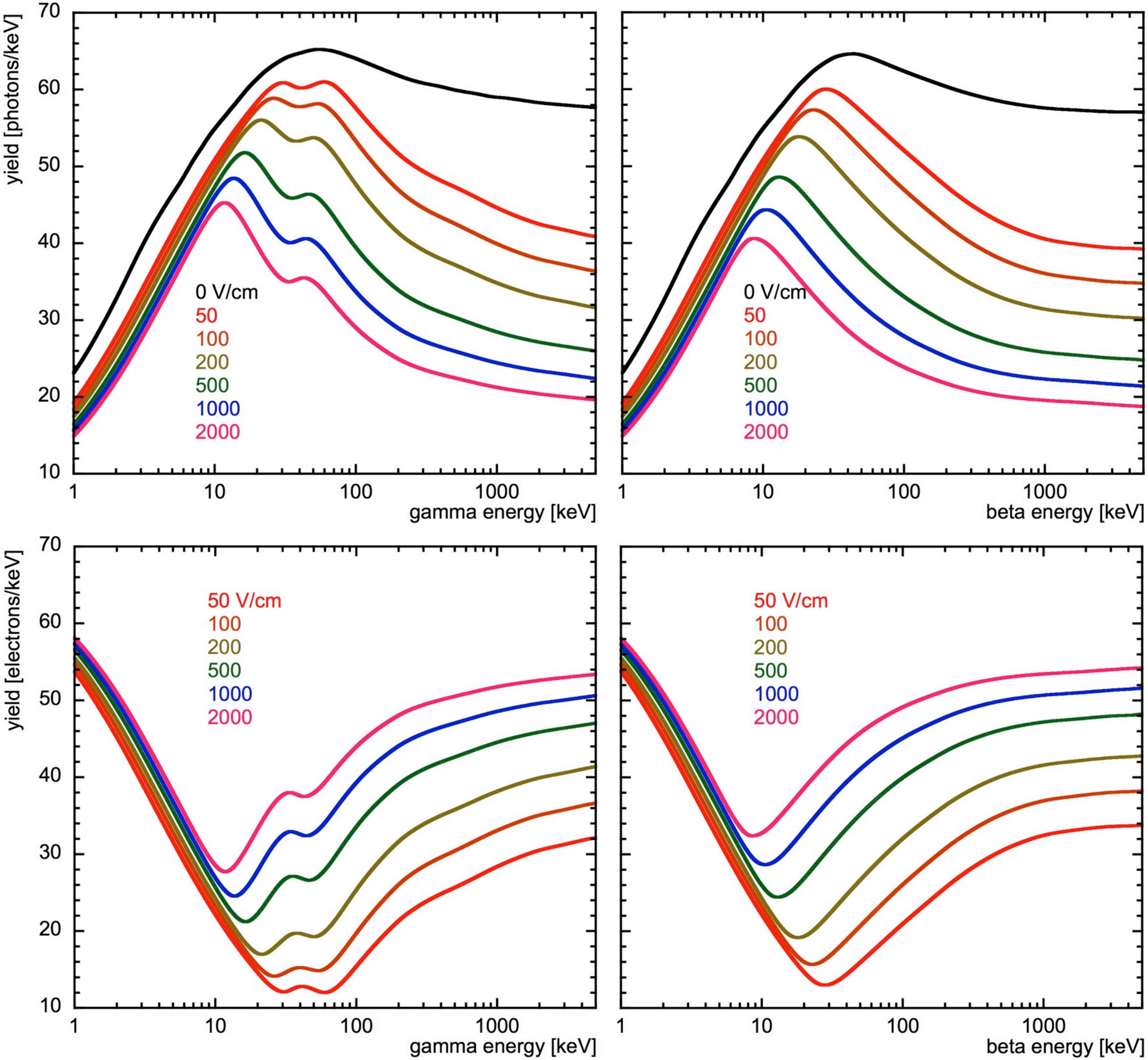


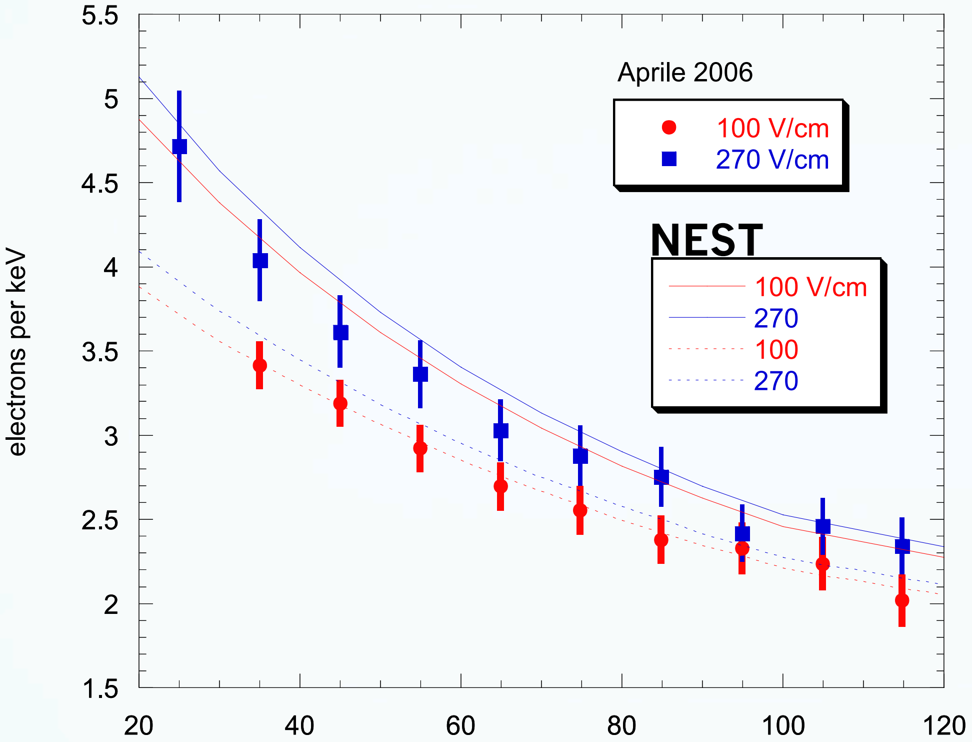
Amoruso et al., NIM A 523 (2004) pp. 275–286

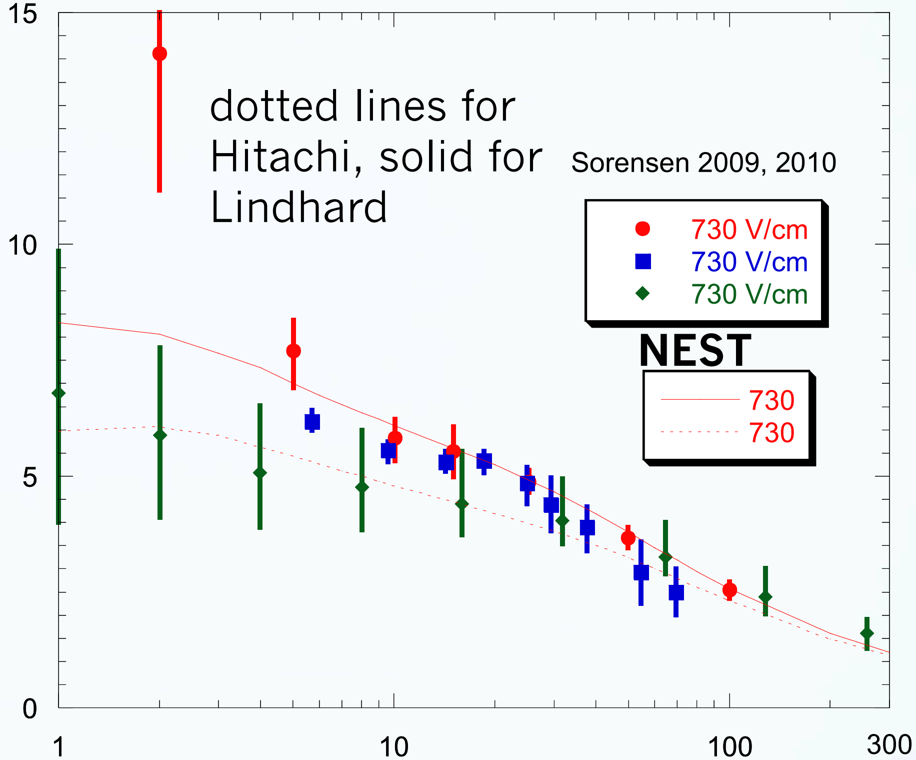
CONCLUSIONS

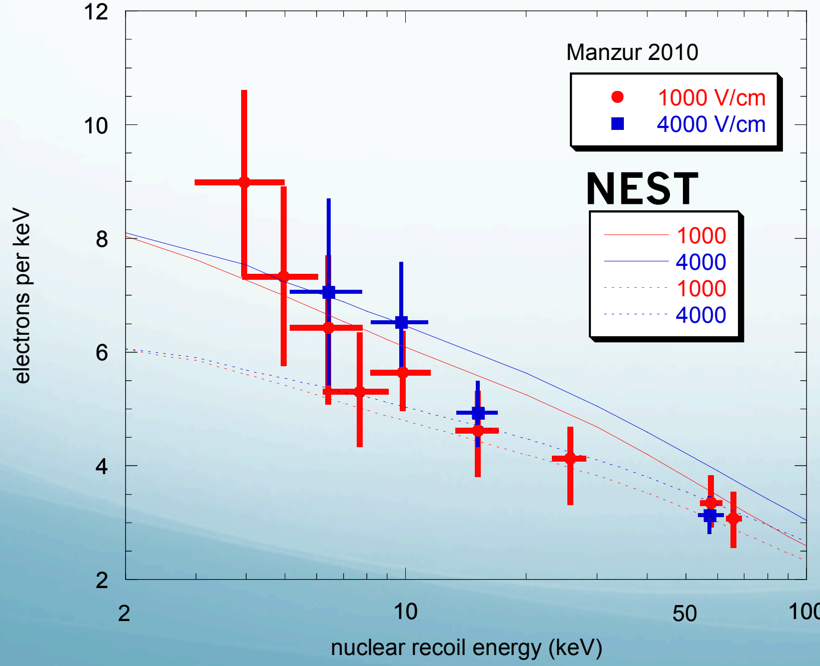
- Simulation model and code NEST has a firm grasp of noble microphysics, at least for liquid xenon
- Though NEST does not track individual atoms or excimers, it is close to first principles, considering the excitation, ionization, and recombination physics, resorting to empirical interpolations as indirect fits, or not all
- Extensive empirical verification against past data undertaken using multiple papers
- Liquid xenon is essentially finished, but there is still work being done for liquid argon
- User-editable code for the entire community
- Our understanding of the microphysics is only as good as the best data. Models are beautiful but nature is tricky. NEST is constantly improving.

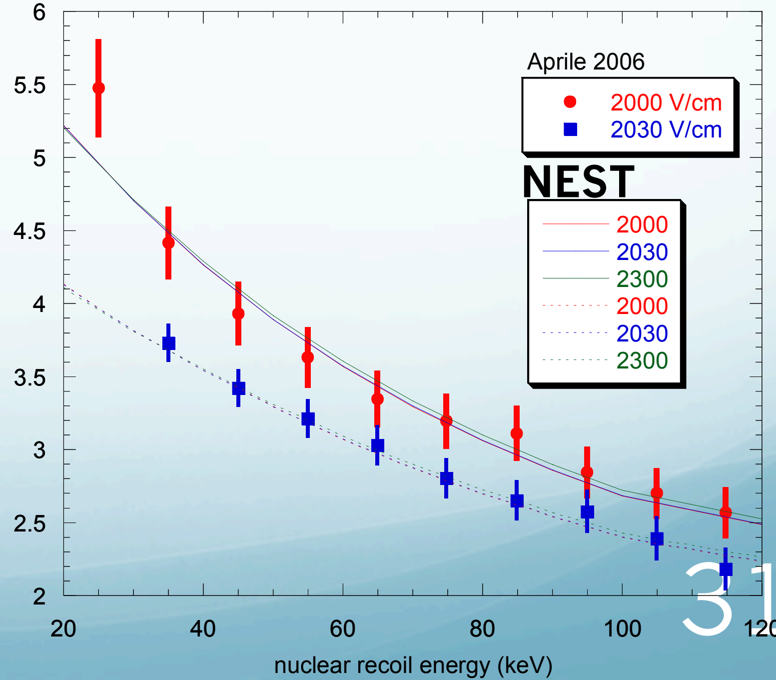

residual (%)
4
0
-4
absolute yield (photons/keV)
80
75
70
65
60
55
50
effective work function W_{ph} (eV)
12.5
13.3
14.3
15.4
16.7
18.2
20.0
1
10
100
1000
10^4
incident gamma energy (keV)
This Work
best reproduction based on model
Doke/Birks' Law only
Thomas-Imel box model only
Barabanov (1987)
Bolozdynya (2008)
Chepel (1999)
Dahl (2009)
Manalaysay (2010)
Ni (2006)
Ni (2007)
Obodovskii (1994)
Shutt (2007)
Yamashita (2003)
Yamashita (2004)
Doke (2001) Calculation
(Not to be confused with Doke/Birks' Law)


yield [photons/keV]
70
60
50
40
30
20
10
0 V/cm
50
100
200
500
1000
2000
1
10
100
1000
gamma energy [keV]
beta energy [keV]
yield [electrons/keV]
50 V/cm
100
200
500
1000
2000
gamma energy [keV]
beta energy [keV]

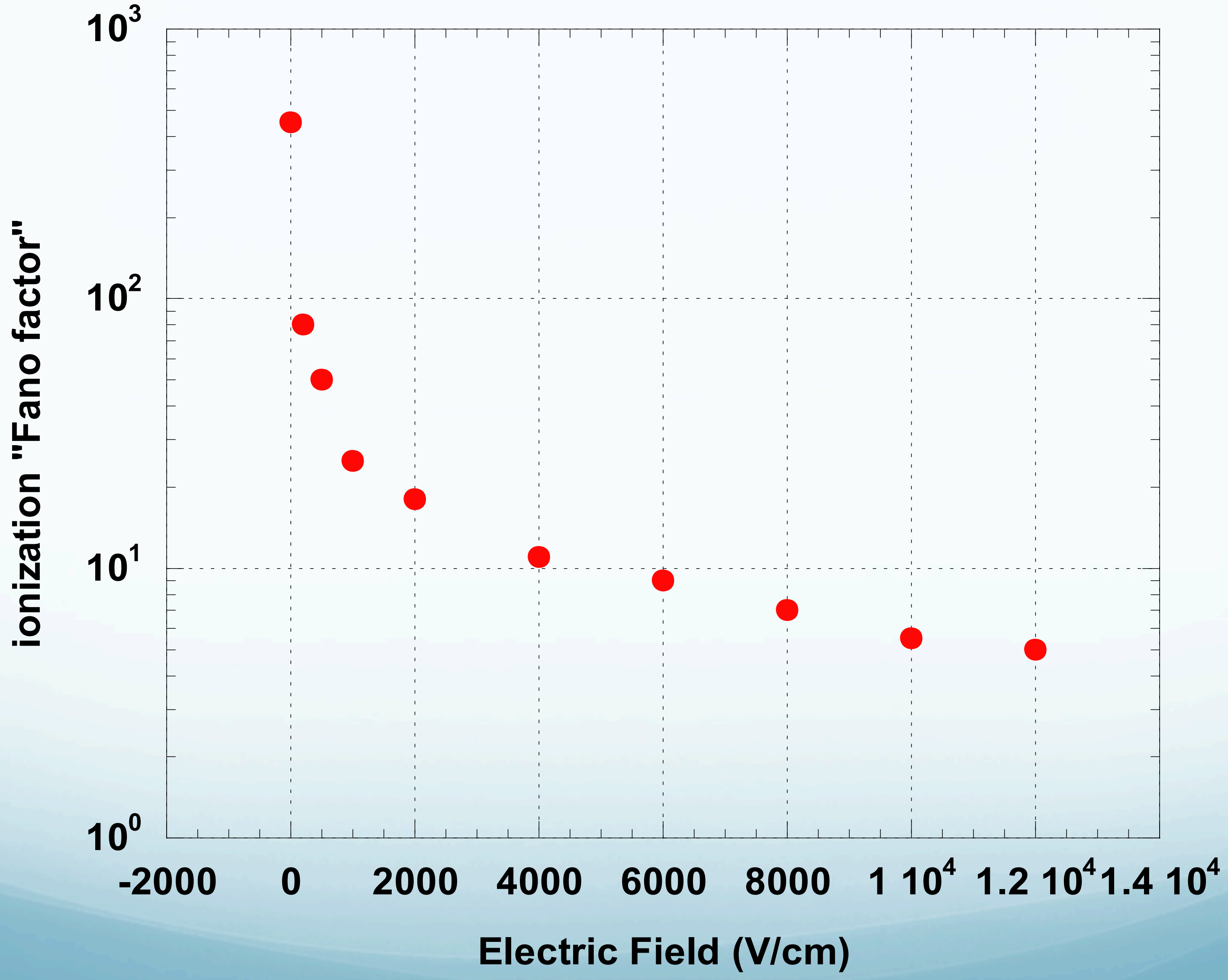



dotted lines for Hitachi, solid for Lindhard

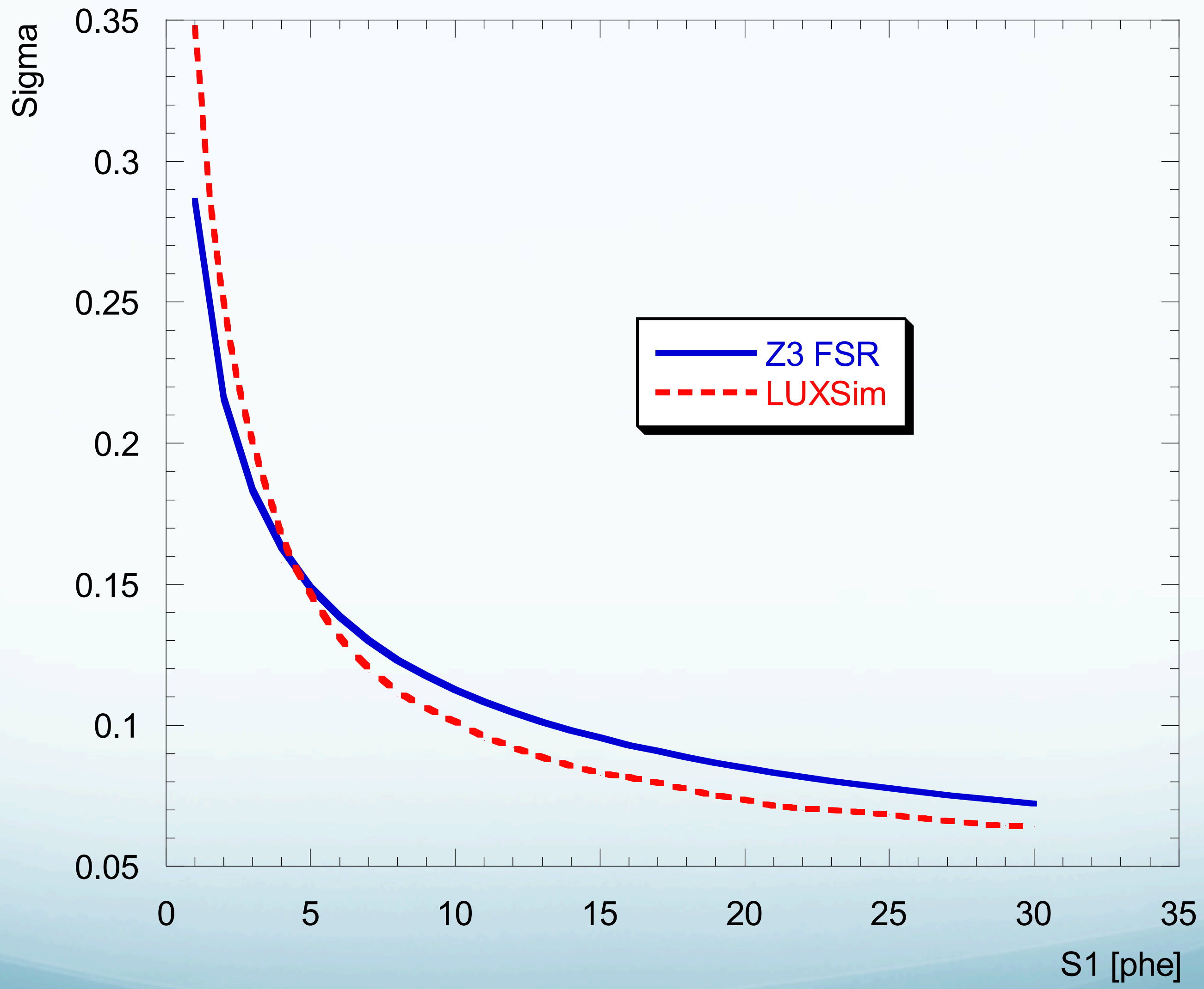




The Recombination Fluctuations



ZEPLIN-III Band Width



Variation in L-Factor