A Symphony of Scintillation

Noble **E**lement **S**imulation **T**echnique, MC Code for Both Scintillation and Ionization in Noble Elements.

http://nest.physics.ucdavis.edu

Matthew Szydagis

M. Szydagis, N. Barry, K. Kazkaz, J. Mock, D. Stolp, M. Sweany, M. Tripathi, S. Uvarov, N. Walsh, and M. Woods, "NEST: A Comprehensive Model for Scintillation Yield in Liquid Xenon," *JINST* **6** P10002 (2011). e-Print version: arxiv:1106.1613v1 [physics.ins-det]

Light Detection in Noble Elements, Fermilab, Wednesday 05/29/2013

The People of the NEST Team

UC Davis and LLNL

A small but passionate group of individuals who love their work

<u>Faculty</u>

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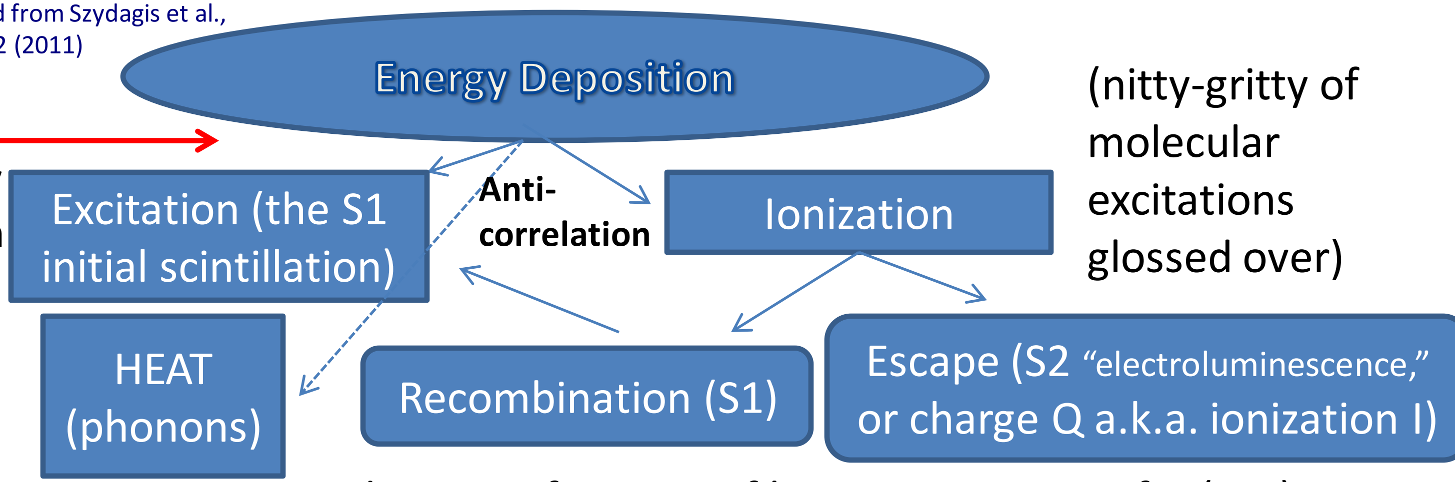
UC Davis undergraduates and summer REU students (many)

What is NEST?

- That name refers to both a model (or, more accurately, a collection of models) explaining the scintillation and ionization yields of noble elements as a function of particle type (ER, NR, alphas), electric field, and energy or dE/dx
- … as well as to the C++ code for GEANT4 that implements said model(s), overriding the default
- Goal is to provide a full-fledged MC sim with
  - Mean yields (light AND charge)
  - Energy resolution (and background discrimination)
  - Pulse shapes (S1 AND S2)
- Combed the wealth of data for liquid and gaseous noble elements and combined everything learned
- We cross boundaries: ν's, DM, HEP, "enemies"

Basic Physics Principles

Image adapted from Szydagis et al., *JINST* **6** P10002 (2011)



(nitty-gritty of molecular excitations glossed over)

1st division of energy deposition a function of interaction type (nuclear vs. e-recoil) but not particle type (e.g., e-,γ same), and (~) not a function of the parent particle’s initial kinetic energy

(infamous “quenching” factor, NR)

division a function of linear energy transfer (LET) or stopping power (dE/dx), because of ionization density considerations, and of the electric field magnitude

- The ratio of exciton to ion production is O(0.1)
- S1 is NOT E, because energy depositions divide into 2 channels, S1 and S2, non-linearly: idea from Eric Dahl
- Nuclear recoils also have to deal with Lindhard*

* but it affects BOTH charge and light production

Basic Physics Principles

- Cornerstone: There is but ONE work function for production of EITHER a scintillation photon or an ionization electron. All others derive from it.
- W_{LXe} = 13.7 +/- 0.2 eV $N_q = (N_{e-} + N_\gamma) = E_{dep} / W$

  C.E. Dahl, Ph.D. Thesis, Princeton University, 2009
- $N_\gamma = N_{ex} + r N_i$ and $N_{e-} = (1 - r) N_i$ (N_{ex} / N_i fixed)
- Two recombination models, short and long tracks
  - Thomas-Imel "box" model (below O(10) keV)
  - Doke's modified Birks' Law Doke et al., NIM A 269 (1988) p. 291

volume/bulk or columnar recombination

$$r = \frac{A\frac{dE}{dx}}{1 + B\frac{dE}{dx}} + C, \quad B = A/(1-C) \quad \textbf{OR} \quad r = 1 - \frac{\ln(1+\xi)}{\xi}, \quad \xi \equiv \frac{N_i \alpha'}{4a^2 v}$$

geminate (parent ion)

- Probability r makes for a non-linear yield per keV

Comparison With Data

- Reviewing only NEST's "greatest hits" here, demonstrating not only its post-dictions but also its predictive power for new data, but only scratching the surface in 20 minutes ….
- At non-zero field, NEST based primarily on the Dahl thesis
  - His data extensive in field (.06 to 4 kV/cm) and energy (~2+ keV)
  - Dahl attempted to reconstruct the original, absolute number of quanta and estimate the *intrinsic* resolution you can't avoid
  - Used combined energy, possibly the best energy estimator
- After models built from old data sets, everything else is a prediction of new data, and NOT a fit / spline of data points

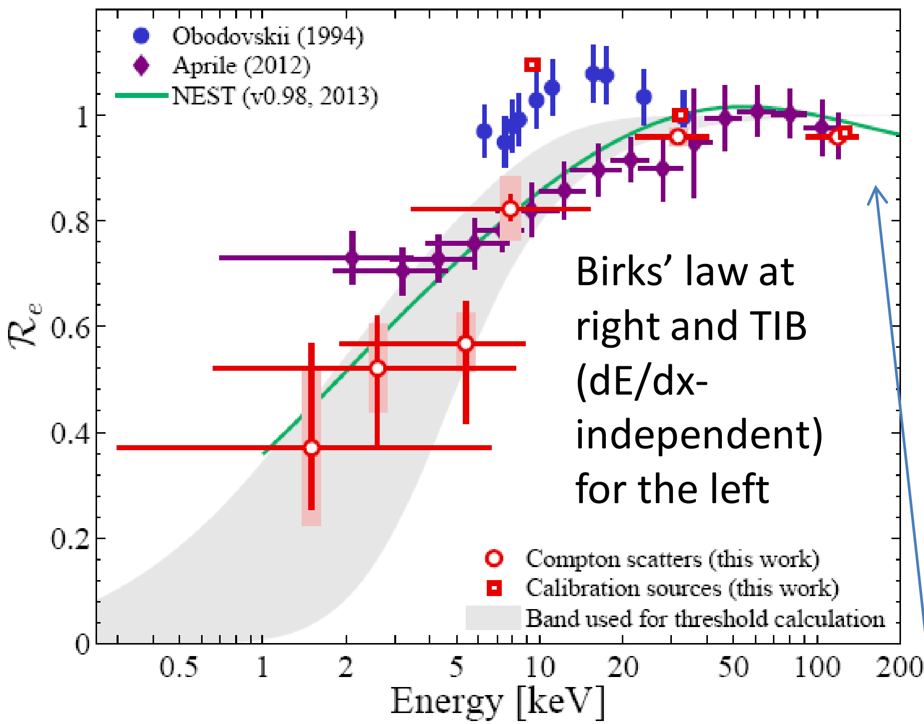
- NEST paper (JINST) contains over 70 references (some rare)
- Going against long-standing assumptions from years back: for example, yield NOT flat versus energy, at least for LXe. No such thing as a generic 'ER' curve. I dug up old papers long forgotten. The ancient results come back in cycles ….

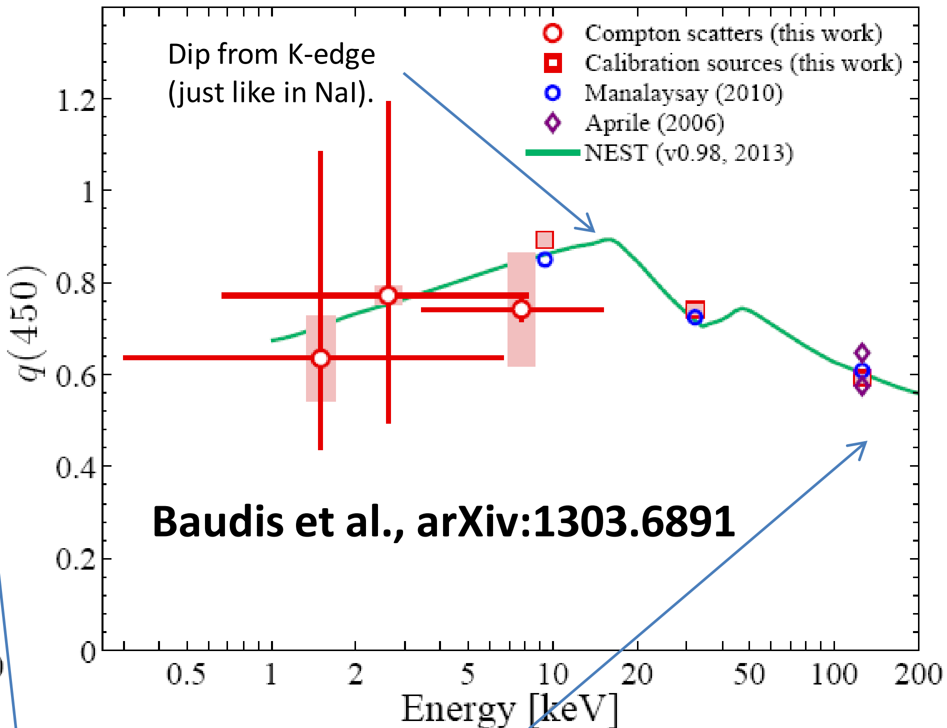
ER Mean Light Yield in LXe

(See Aaron Manalaysay's talk)

Zero Field

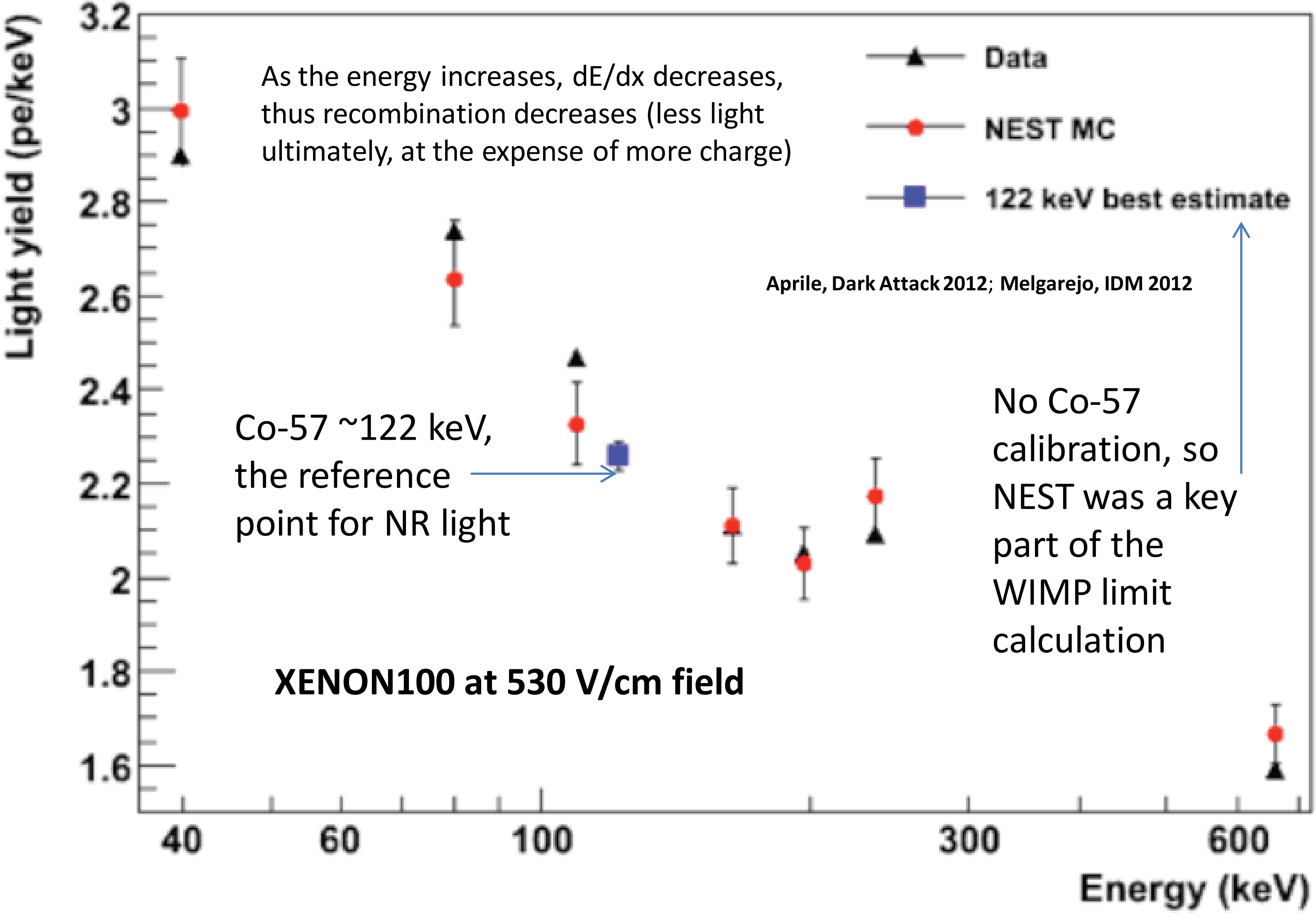
Non-zero Field (450 V/cm)



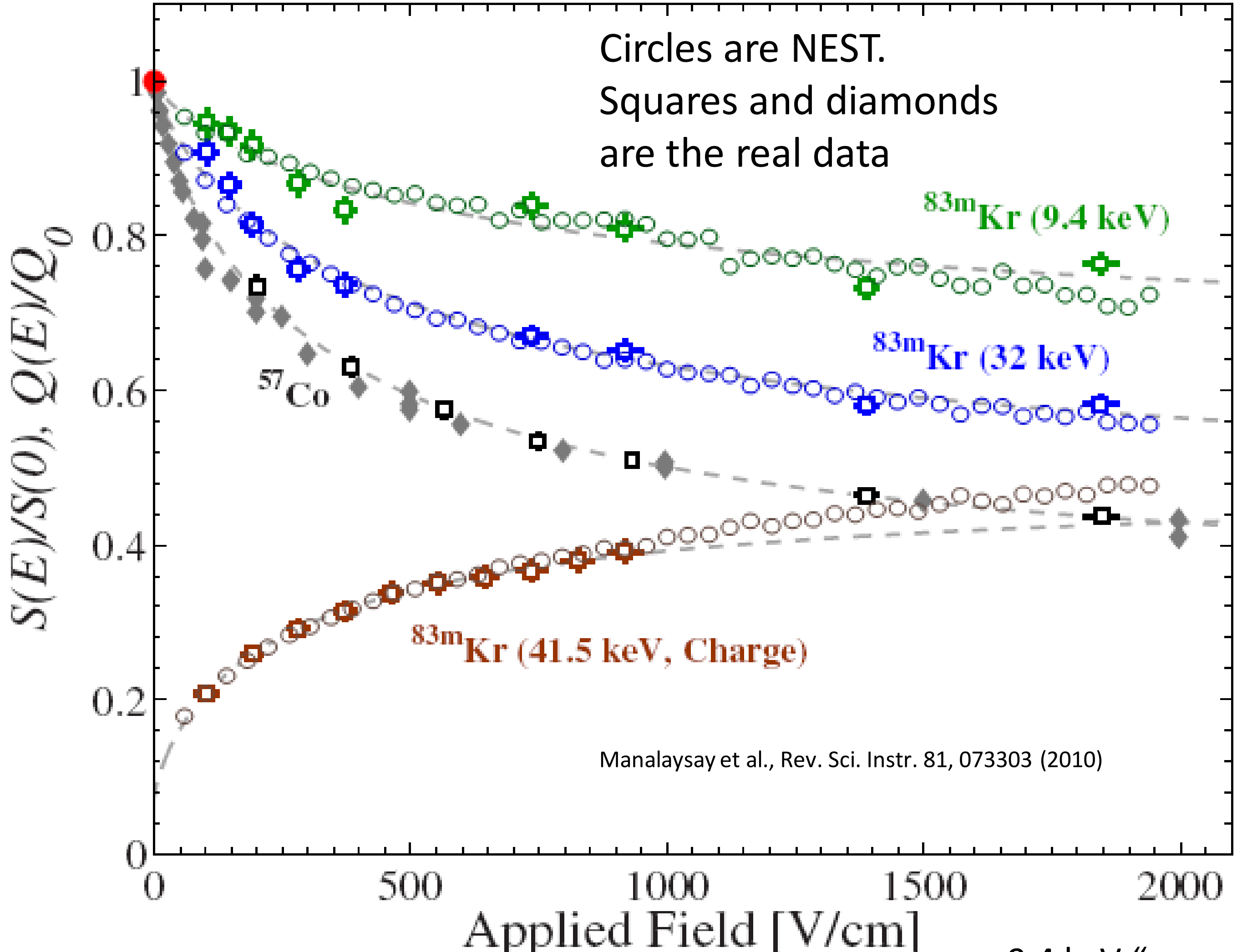


As we approach minimally-ionizing, the curve asymptotes

ER Mean Light Yield in LXe



ER Charge Yield, including Kr-83m



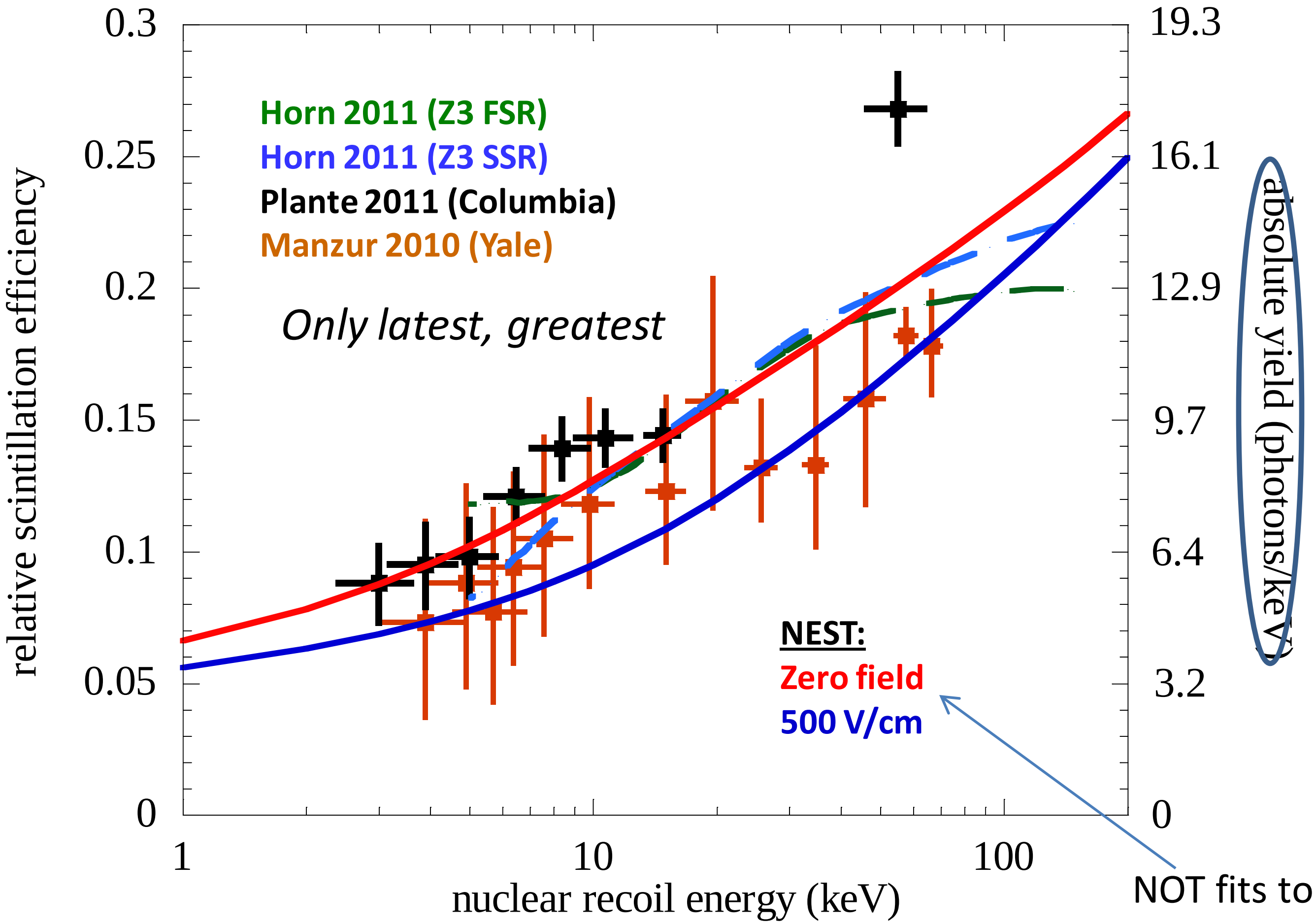
(NEST curve not shown for ^{57}Co because tautology: basis of model)

have benefited from technological advancements, leading to more accurate measurements. Recent 9.4 keV data is poorly predicted by the Thomas-Imel model. Curiously, agreements can be achieved by approximating the ^{83m}Kr de-excitation as only a gamma ray and applying the Doke/Birks model despite the low energy. Without such adjustments these data contradict Dahl [11] in this energy

9.4 keV “anomaly” was identified in the NEST JINST paper ~1 year before Columbia study

NR Light Yield in LXe

(Using very simple assumptions)

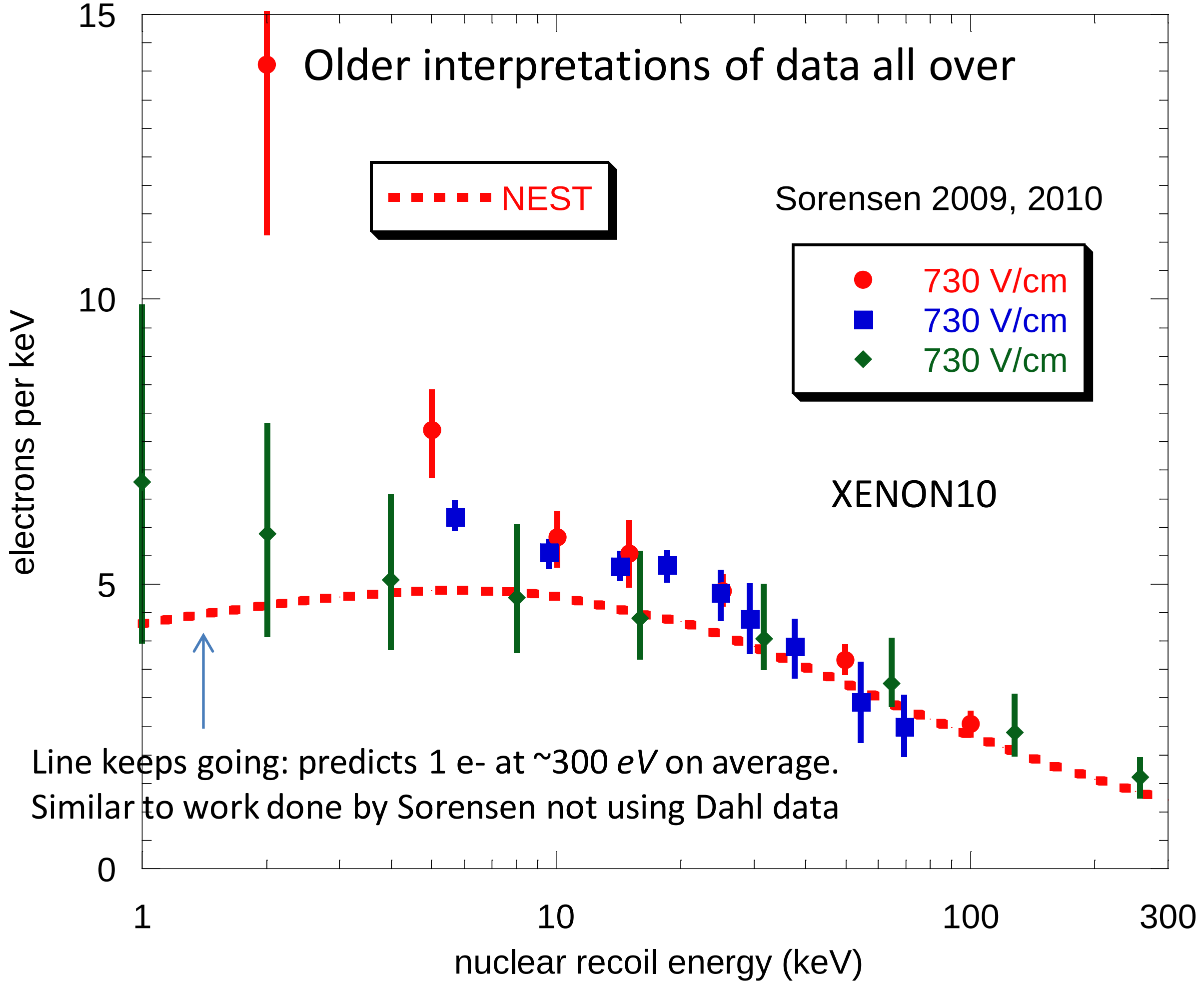


We don't need to reference the 122 keV gamma line anymore. Model gives us absolute numbers.

NOT fits to these data

NR Charge Yield in LXe

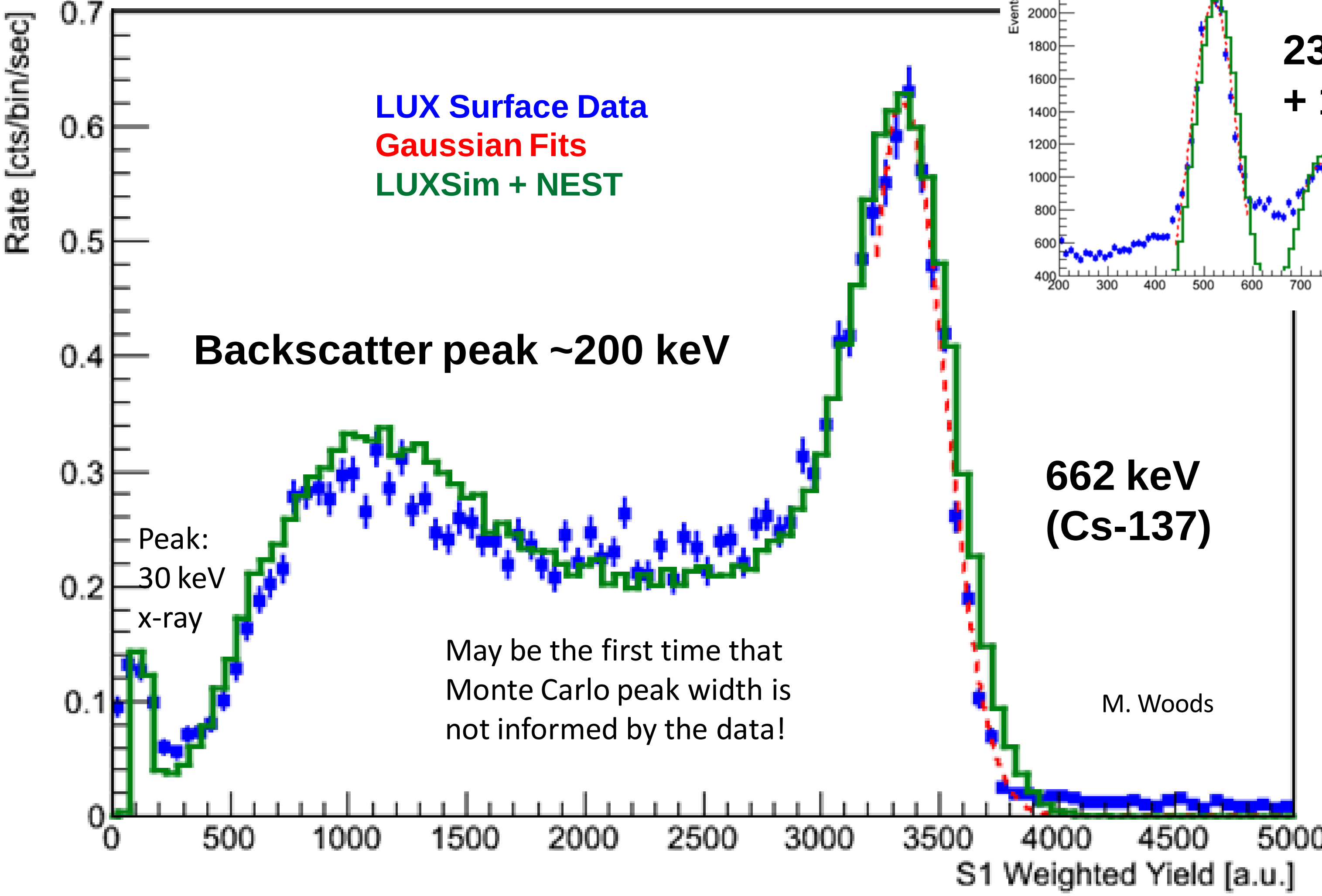
This curve straight-jacketed: sum of quanta fixed by Lindhard theory, while Dahl gives us the ratio



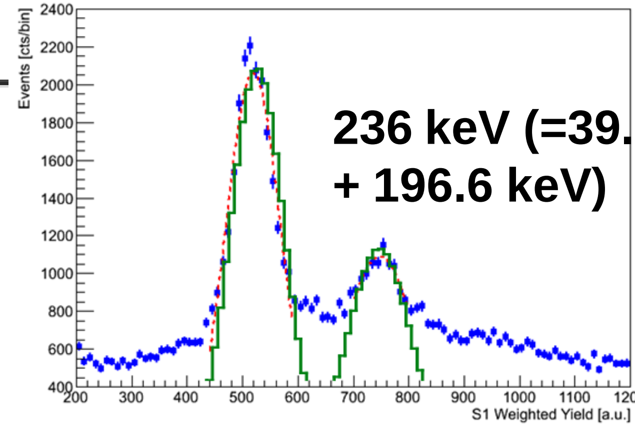
P. Sorensen et al., Lowering the low-energy threshold of xenon detectors, PoS (IDM 2010) 017 [arXiv:1011.6439].

ER Energy Resolution: Light

D. S. Akerib et al., "*Technical Results from the Surface Run of the LUX Dark Matter Experiment*," *Astropart. Phys. 45 (2013) pp. 34-43* arXiv:1210.4569



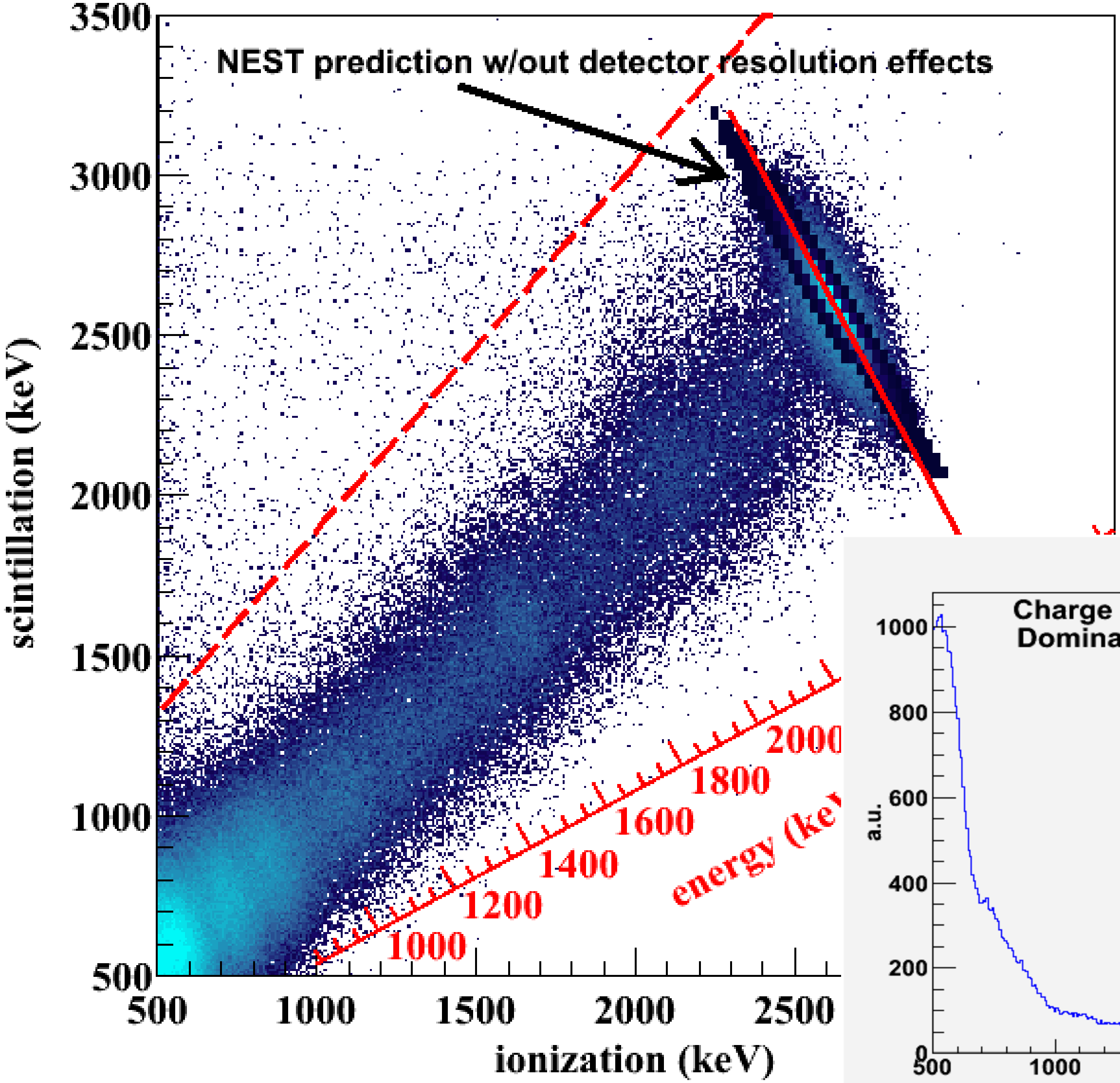
164 keV



236 keV (=39.6 + 196.6 keV)

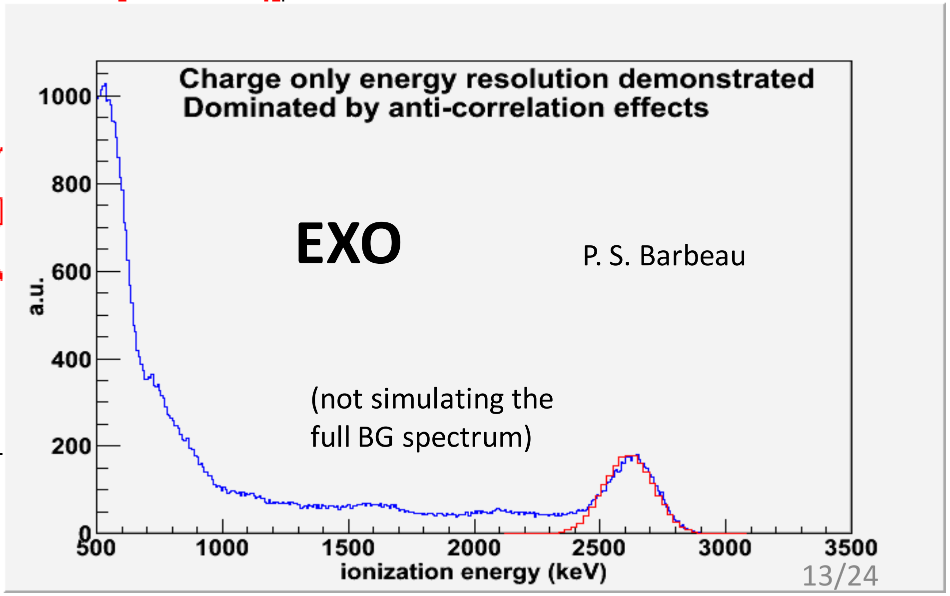
Cosmo-genically activated Xenon

ER Resolution: Charge + Light



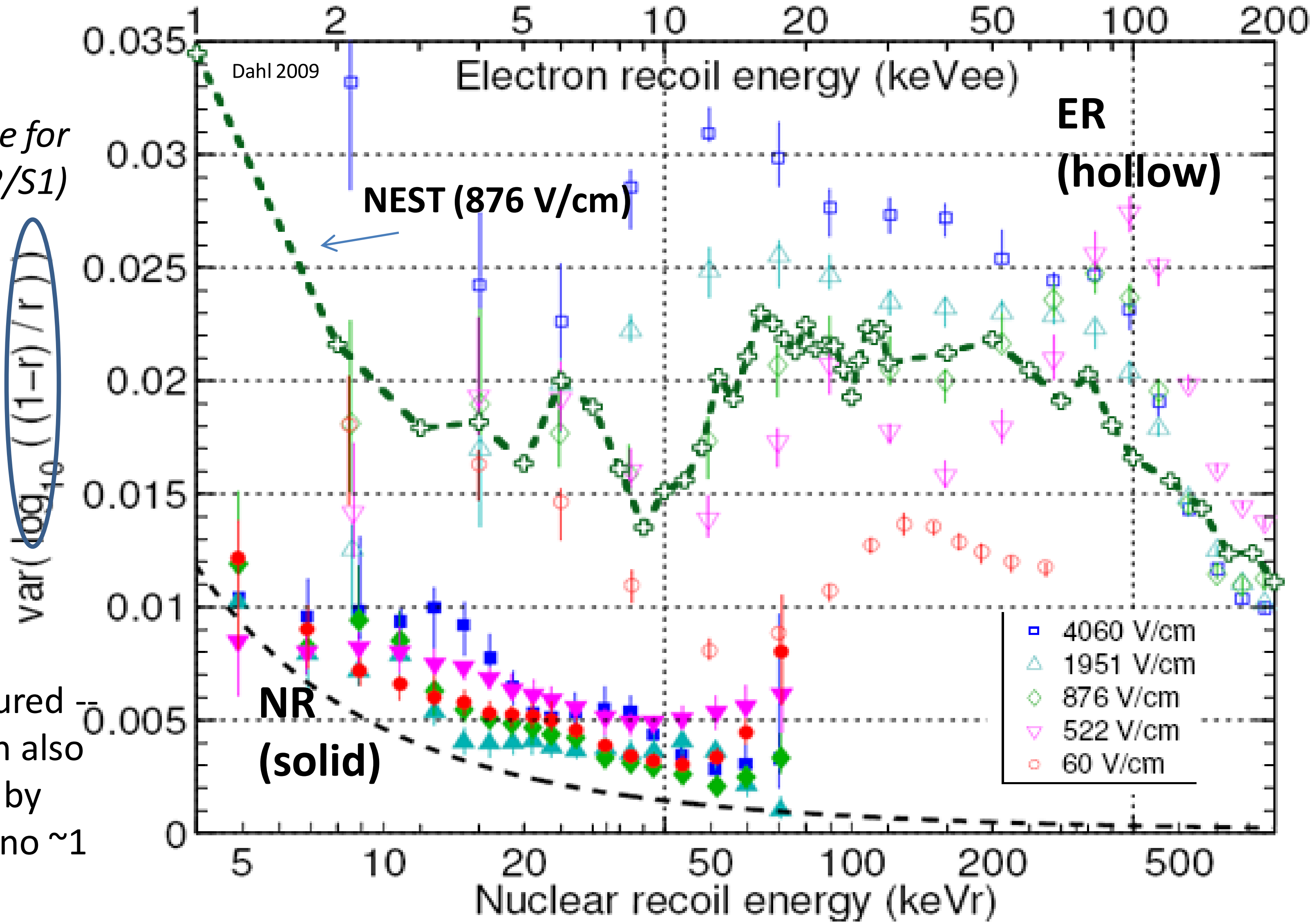
The recombination fluctuations have been modeled as worse than binomial, with a field-dependent Fano-like factor O(10)-O(100) which disappears at low energies. Based on

Conti et al., Phys. Rev. B 68, 054201 (2003)
Aprile et al., NIM A 302, p. 177 (1991)



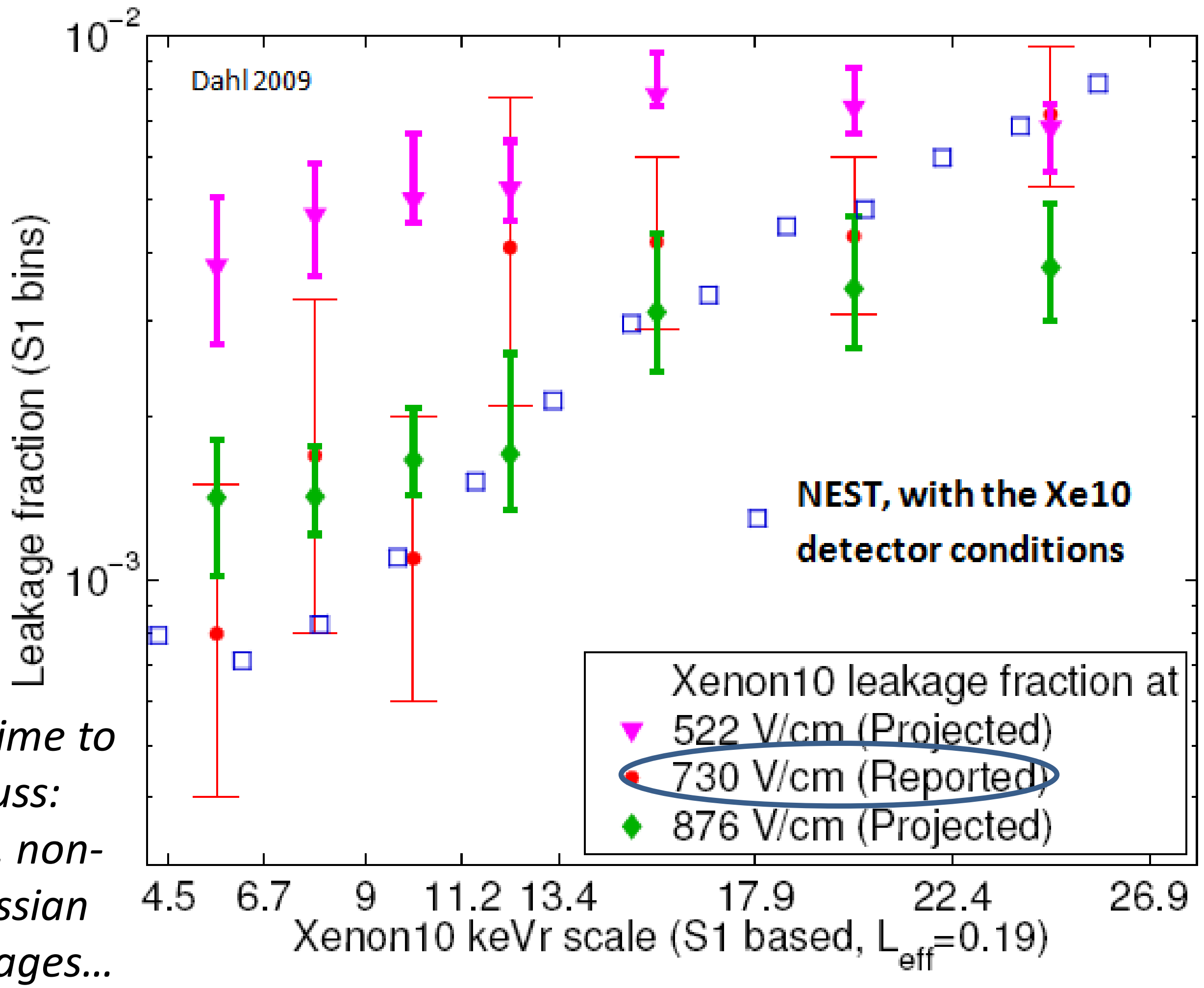
ER Resolution: log(S2/S1) Band

Analogue for log10(S2/S1)



Not pictured -- NR width also handled by NEST: Fano ~1

NR vs. ER Discrimination

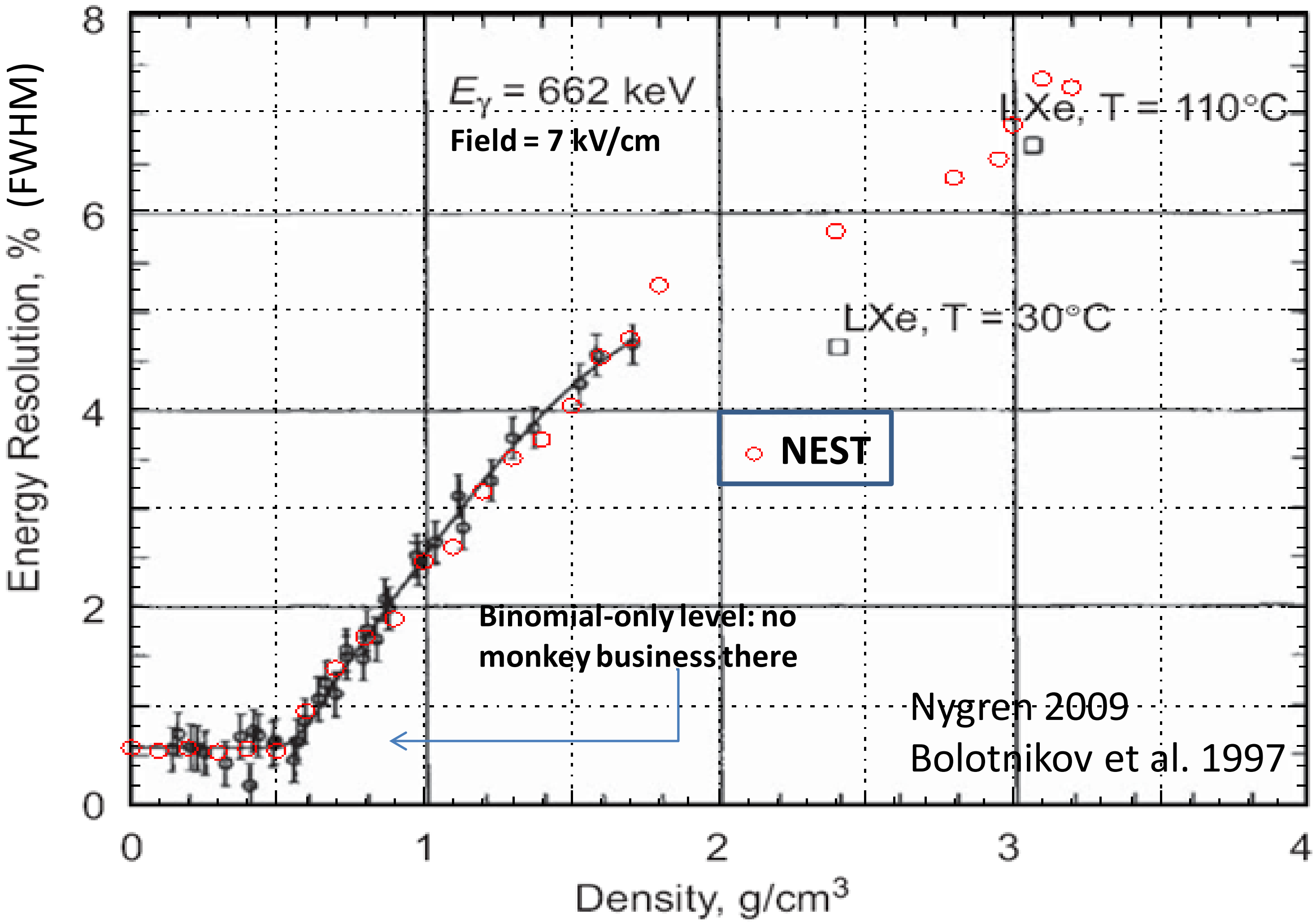


Culmination plot. ER and NR band means and widths must all be correct. The trend is counter-intuitive: worse result *away* from threshold.

No time to discuss: tails, non-Gaussian leakages…

Gaseous Xenon

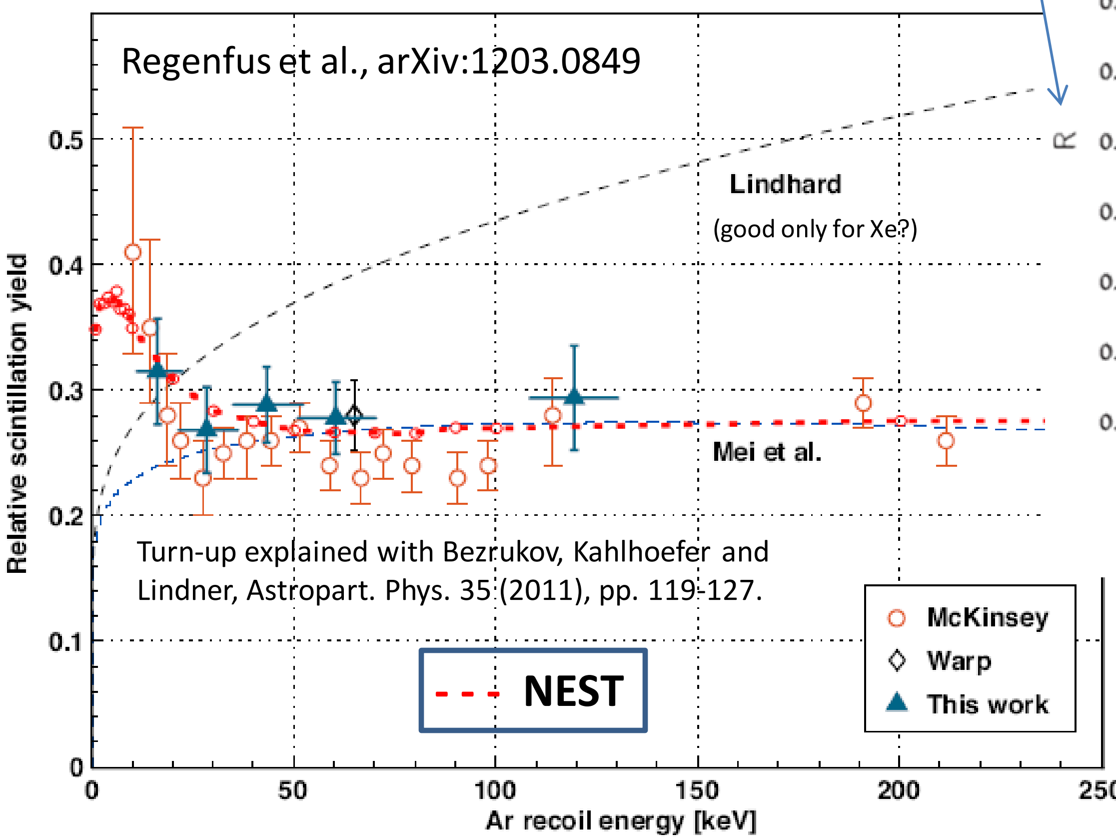
(The mystery of liquid's worse energy resolution)

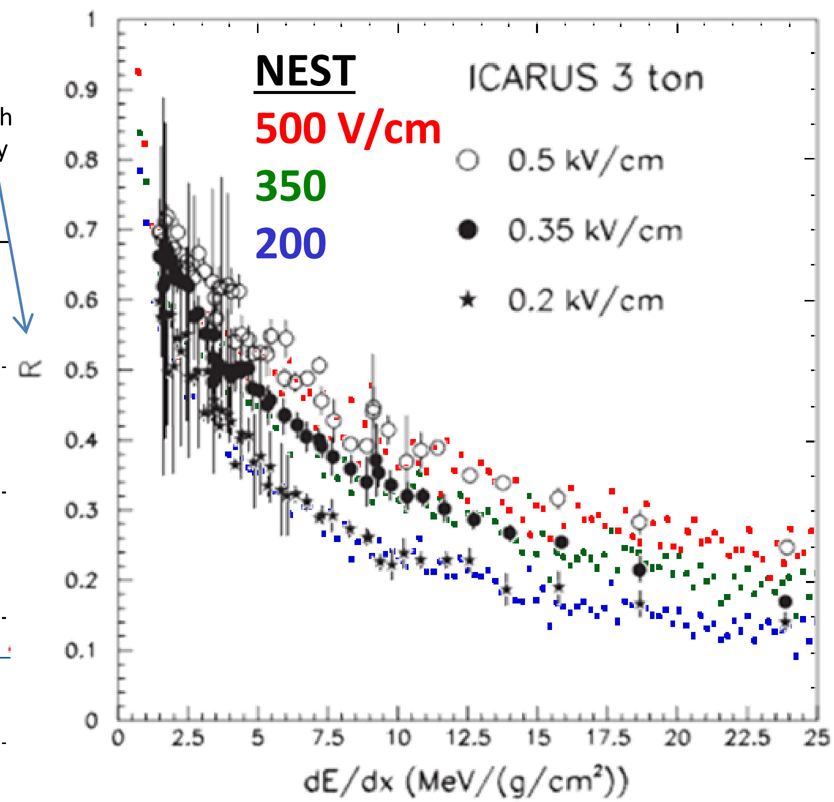


Liquid Argon NR and ER

Note: RAT, codebase pre-dating NEST, already does zero-field LAr very well (talk with S. Seibert)

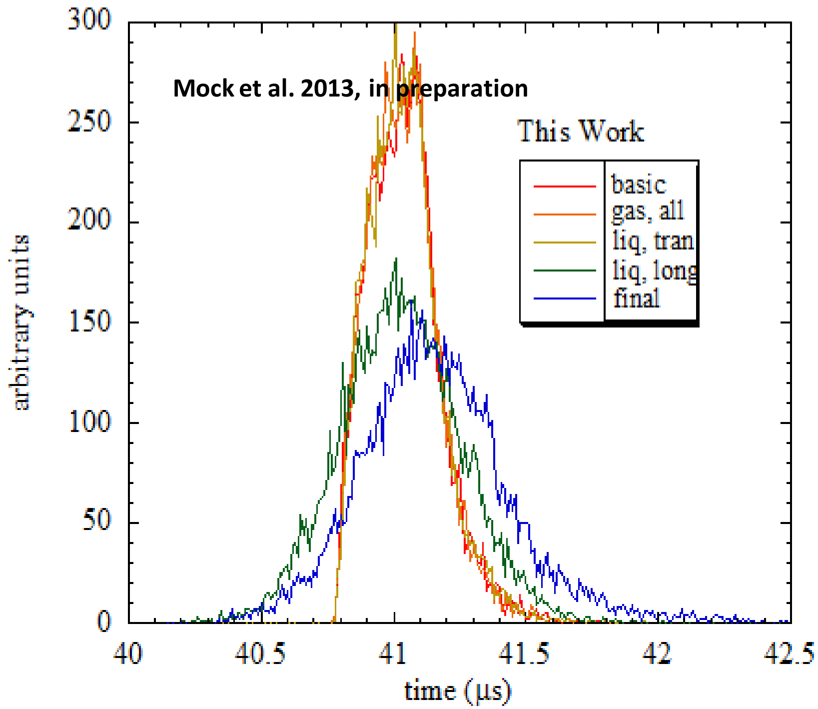
R = 1 –r is a way of checking on both light and charge yields, concurrently

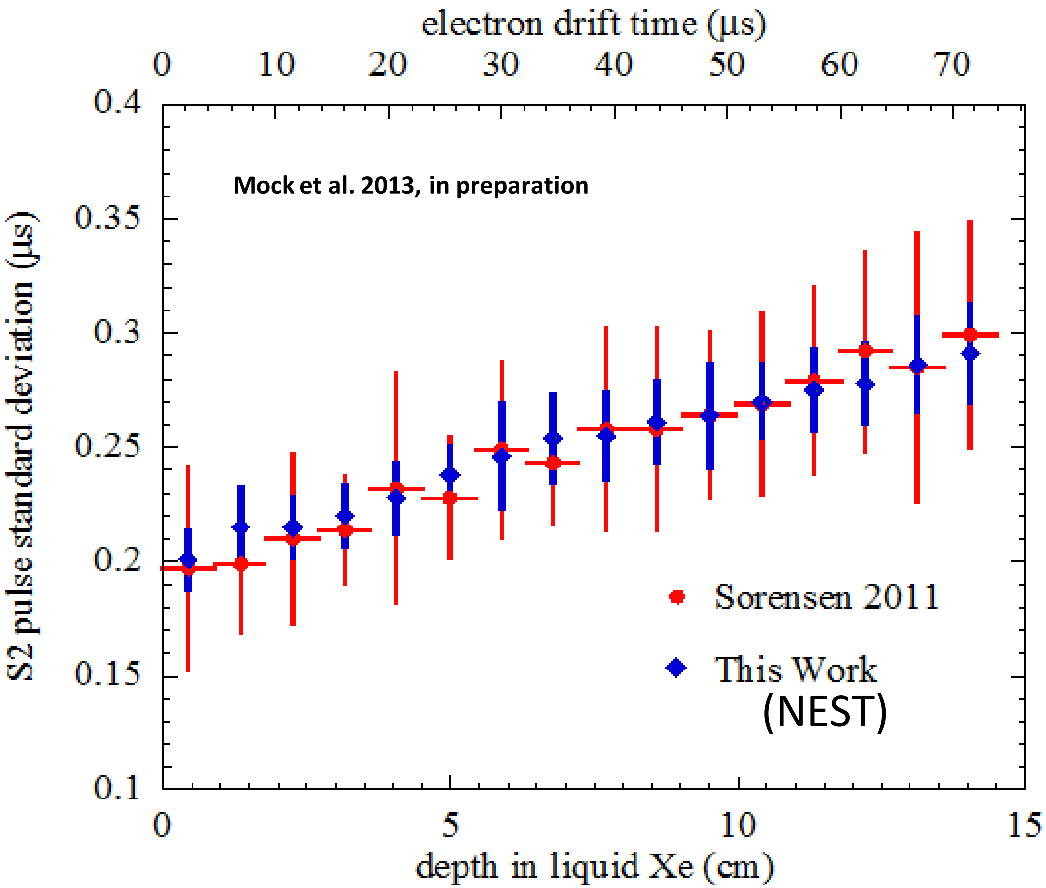


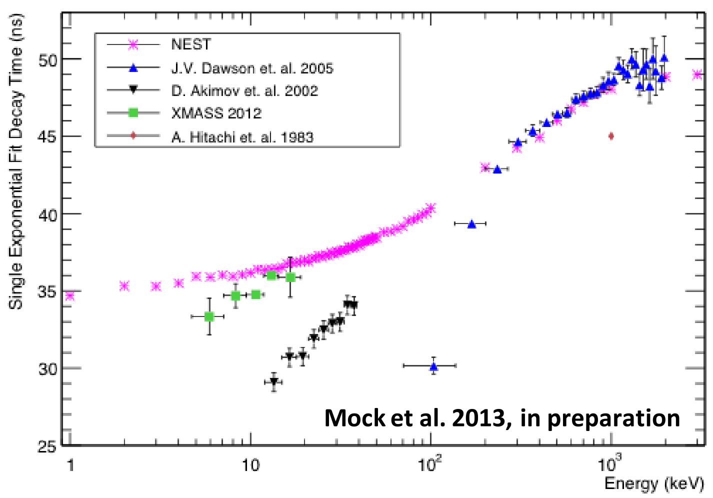


Amoruso et al., NIM A 523 (2004) pp. 275–286

Pulse shape: LXe examples







+ S1 effects included: a singlet time, triplet time, ratio (function of particle type), non-exponential recombination time (function of dE/dx and field)
+ S2 effects: drift speed, singlet, triplet, diffusion, and electron trapping prior to extraction.

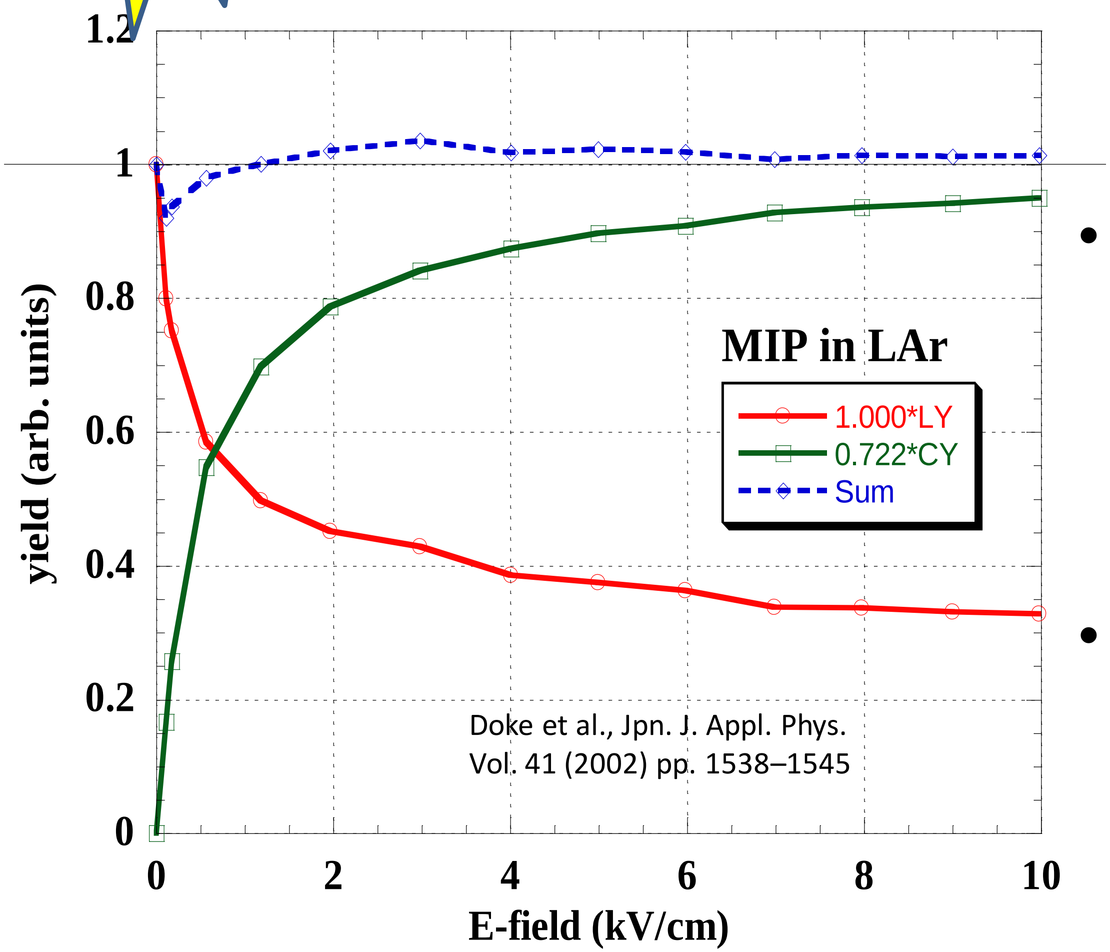
Conclusions

- Simulation package NEST has a firm grasp of microphysics.
- **Though NEST does not track individual atoms or excimers, it is closer to first principles, considering the excitation, ionization, and recombination physics, resorting to empirical interpolations as indirect fits or not at all**
- Extensive empirical verification against past data undertaken using multiple papers instead of only one experiment
- Liquid xenon is essentially finished, but there is still work being done for liquid argon, although it is progressing rapidly
- 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 ugly. NEST is constantly improving. Always on look-out for more physical motivations. Currently, all parameters justifiable except for the size of the recombination fluctuations (in liquid xenon).**

Anti-correlation in Argon

Confirmed by DarkSide!
(see the IDM 2012 talk)

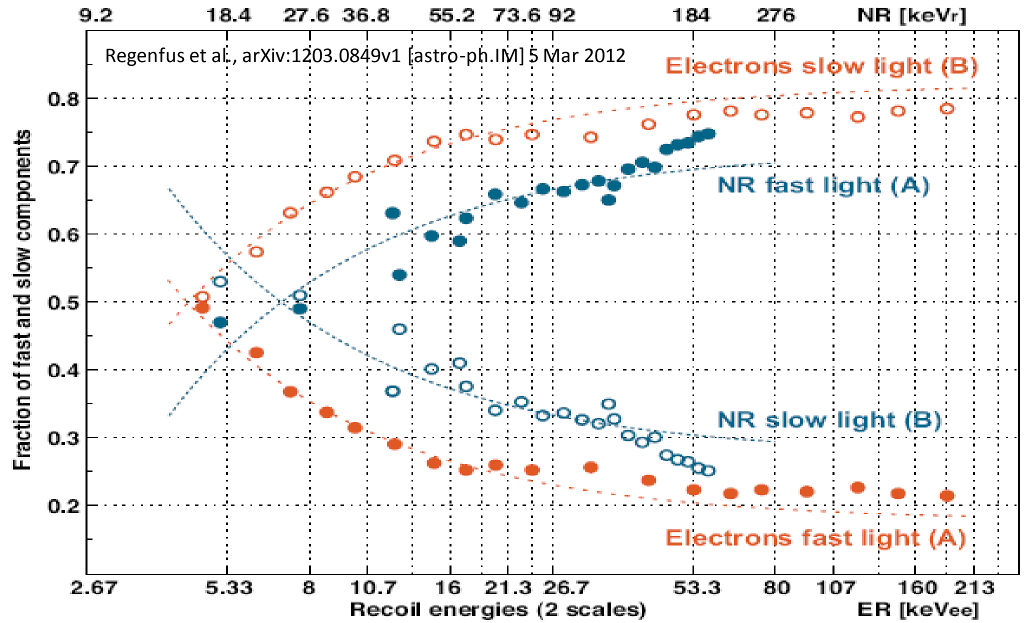
Correct absolute energy scale = *a* * *LY* + *b* * *CY*
(the "constants" *a* and *b* change with electric field and with energy)



- In LAr, anti-correlation between light yield (LY) and charge (CY) missed
- Combining lets you empirically eliminate the effect of recombination fluctuations and energy loss into scintillation
- **In high-light-yield prototype TPCs, we can use mono-energetic sources and sweep the field to test this .....**

LAr Pulse Shape

- The latest version of NEST (98) has incorporated some of these results
- The upper plot has been converted into a function of LET instead of E (soon impurity concentration too)
- This should be a significant step forward in LAr modeling, giving us the correct ratio of triplet to singlet light (it's not flat)



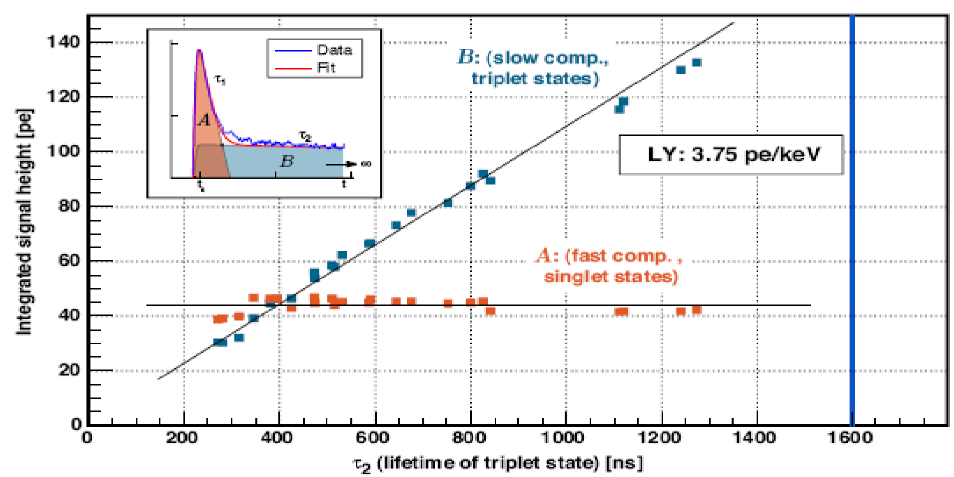
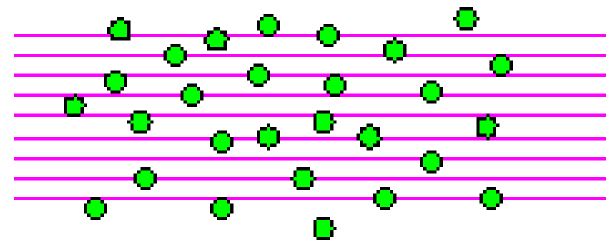


Figure 3. *Yield of the fast and slow scintillation components under different purity conditions.*

Understanding Charge Collection

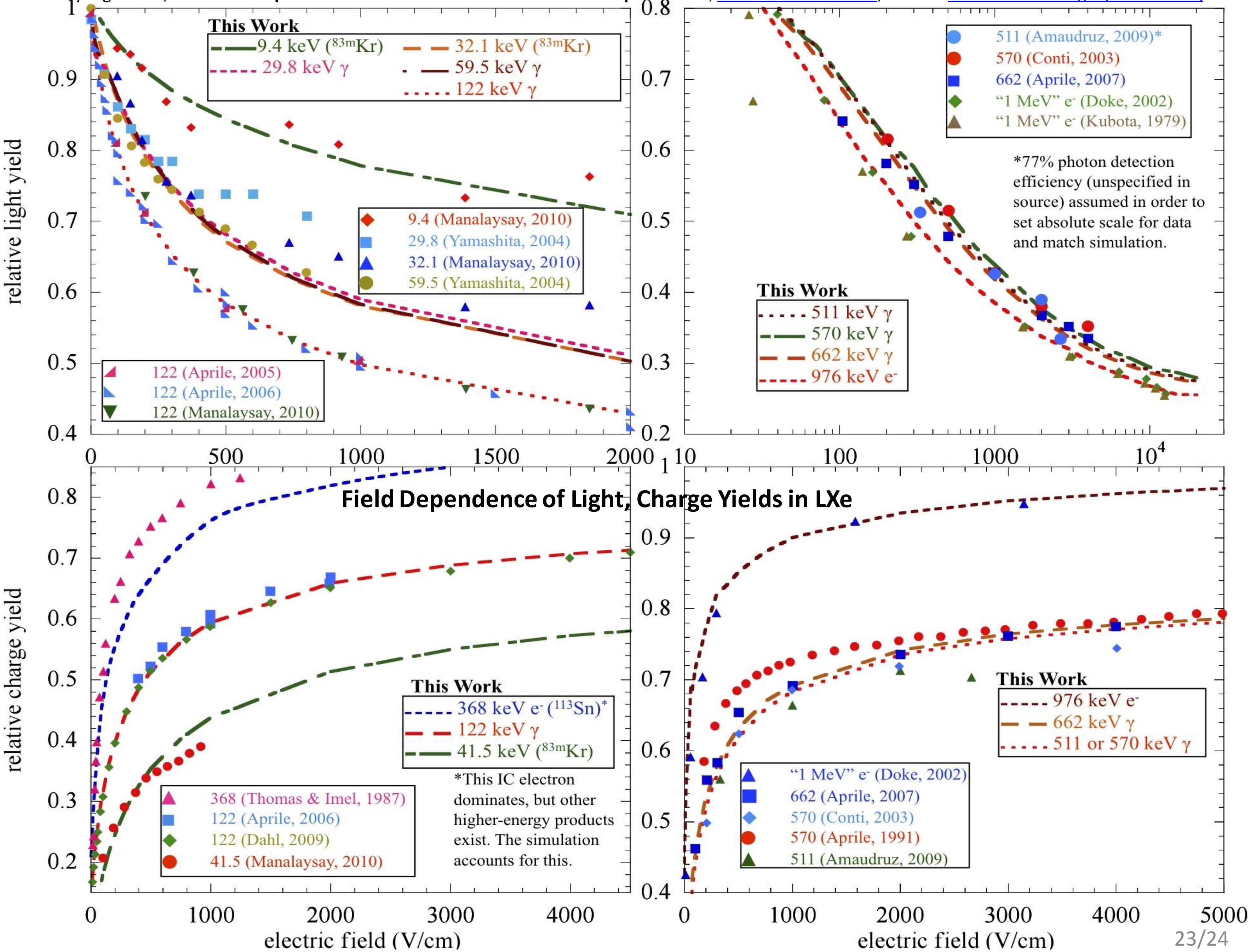


- New G4Particle for drift e-'s
- Analogous to optical photons versus gamma rays
- Normal electrons, if born with tiny energies, are absorbed immediately in GEANT
- Full sims take much longer than parameterized ones, but this new particle (the "thermalelectron") allows tracking of individual ionization sites, and simulated 3-D electric field, purity, and diffusion mapping
- To decrease simulation time, NEST has a built-in feature for charge yield reduction

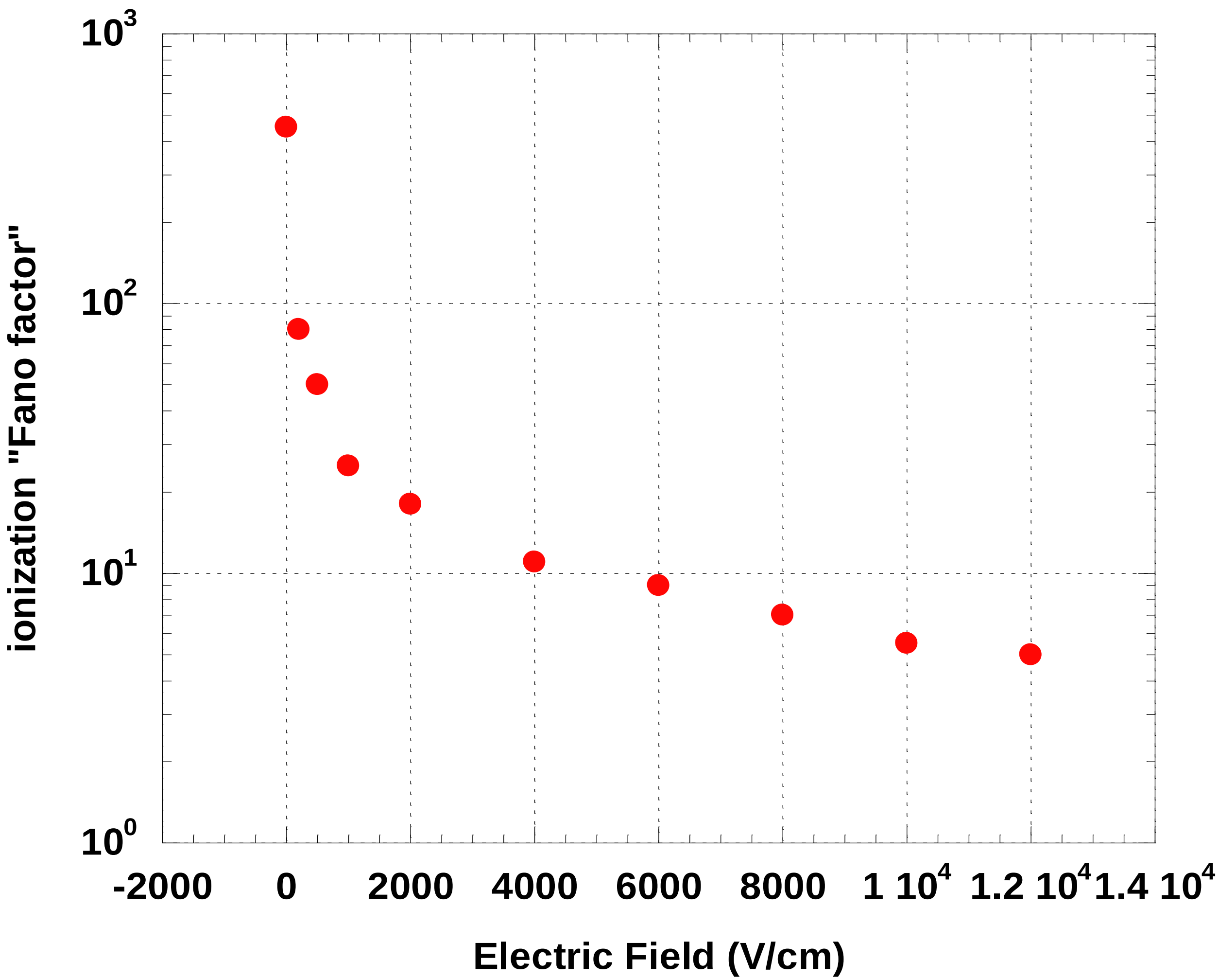
```
*************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 5,   Parent ID = 3
*************************************************************************

Step#    X(mm)    Y(mm)    Z(mm)  KinE(MeV)  dE(MeV)  StepLeng TrackLeng
```

Szydagis et al., **NEST: A Comprehensive Model for Scintillation Yield in Liquid Xenon**, 2011 JINST 6 P10002; e-Print: arxiv:1106.1613 [physics.ins-det]

Field Dependence of Light, Charge Yields in LXe



Recombination Fluctuations Model



- Regular Fano factor left alone
- Recombination fluctuations have been modeled as worse than binomial, with a 1-sigma of sqrt(F_e*N_e), per interaction site
- Field-dependent but energy-independent (except at low E)