A Symphony of Scintillation

Noble **E**lement **S**imulation **T**echnique

for Geant4

http://nest.physics.ucdavis.edu

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on behalf of the entire NEST development team, of the University of California, Davis, Davis, CA, USA, and Lawrence Livermore National Laboratory, Livermore, CA, USA

Shanghai Jiao Tong University, Shanghai, China, Tues., Sept. 20, 2011 @2pm

The People of the NEST Team

UC Davis and LLNL, California

A very small but passionate group of individuals who love this work

Faculty

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Postdocs and Physicists

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Jake Pasner

Graduate Students

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James Morad

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Mike Woods

Why simulate scintillating noble elements well?

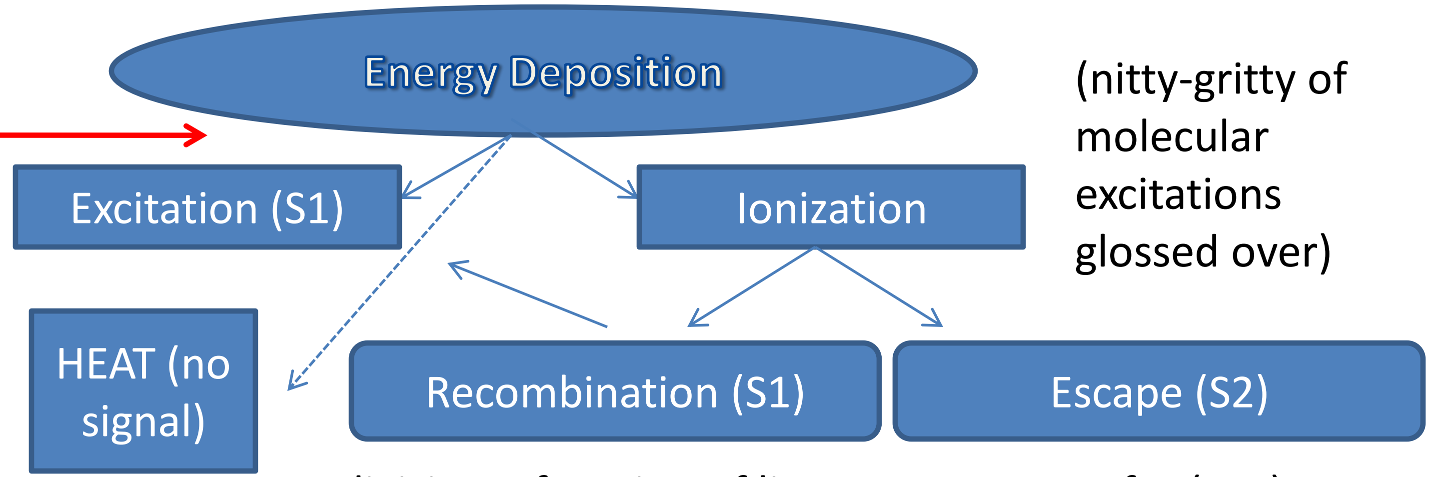
- Direct dark matter detection or calibration for it (past, present, future experiments)
  - LUX, XENON, ZEPLIN, LZ, WArP, DarkSide, ArDM, XMASS, DARWIN, MAX, Xürich, Xed, XeCube, PANDA-X, PIXeY, DEAP, CLEAN, ….. 1- and 2-phase
- Double beta decay ($2\nu\beta\beta$, $0\nu\beta\beta$) projects too
  - EXO, NEXT (both ^{136}Xe-enriched)
- Positron Emission Tomography (PET) scans for medical applications: detect 511 keV γ's
- Other particle detection applications, e.g., collider experiments (MEG, Olive, et al.)

The Purpose and Scope of NEST

- Create a full-fledged simulation based on physical, albeit also heuristic/quasi-empirical approach
- Comb the wealth of data for liquid and gaseous noble elements for different particles, energies, and electric fields, and then combine everything
- Aid the many dark matter, double beta decay, and other experiments which utilize this technology to be on the same or comparable page for simulations
- Bring added realism to the simple model that is present now in Geant4.9.4 for scintillation
- Explore backgrounds at low energy by expanding Geant4 physics to be more accurate when you go to a low energy regime: $O(1)$ keV and even lower
- Have to start somewhere: LXe, for sake of LUX

Basic Physics Principles

(nitty-gritty of molecular excitations glossed over)



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 kinetic energy

(the infamous $\mathscr{L}$ value)

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

- Heat loss for nuclear recoils (Lindhard effect); electron recoils easier to deal with (or are they…?)
- Start simple: no exotic energy loss mechanisms (like "bi-excitonic" collisions). Explains the data?

Model Framework: Start with Electron Recoils

- Look at the Geant4 tracking verbosity: different energy depositions from the secondary electrons and gammas in an EM cascade
- Allow for the recombination% to fluctuate stochastically by treating every electron recoil individually

```
* G4Track Information:   Particle = gamma,   Track ID = 3,   Parent ID = 1
*****************************************************************************************

Step#      X(mm)      Y(mm)      Z(mm)  KinE(MeV)   dE(MeV)  StepLeng  TrackLeng   NextVolume  ProcName
    0     -0.717      -4.18       -141     0.0298         0         0          0  LiquidXenon  initStep
    1      -1.07      -3.87       -141     0.0269  0.000678     0.484      0.484  LiquidXenon  compt
    2      -1.14      -4.18       -140          0   0.00542     0.565       1.05  LiquidXenon  phot

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

Step#      X(mm)      Y(mm)      Z(mm)  KinE(MeV)   dE(MeV)  StepLeng  TrackLeng   NextVolume  ProcName
    0      -1.14      -4.18       -140     0.0215         0         0          0  LiquidXenon  initStep
    1      -1.14      -4.18       -140    0.00877   0.00795   0.00306    0.00306  LiquidXenon  eIoni
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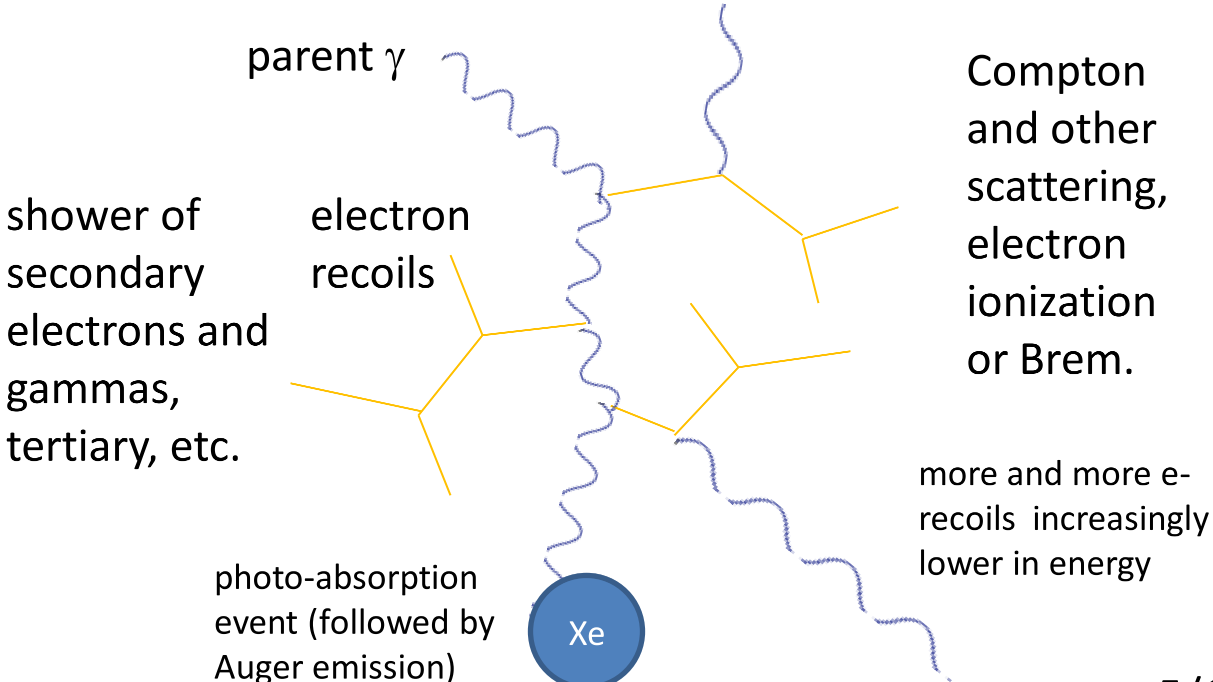
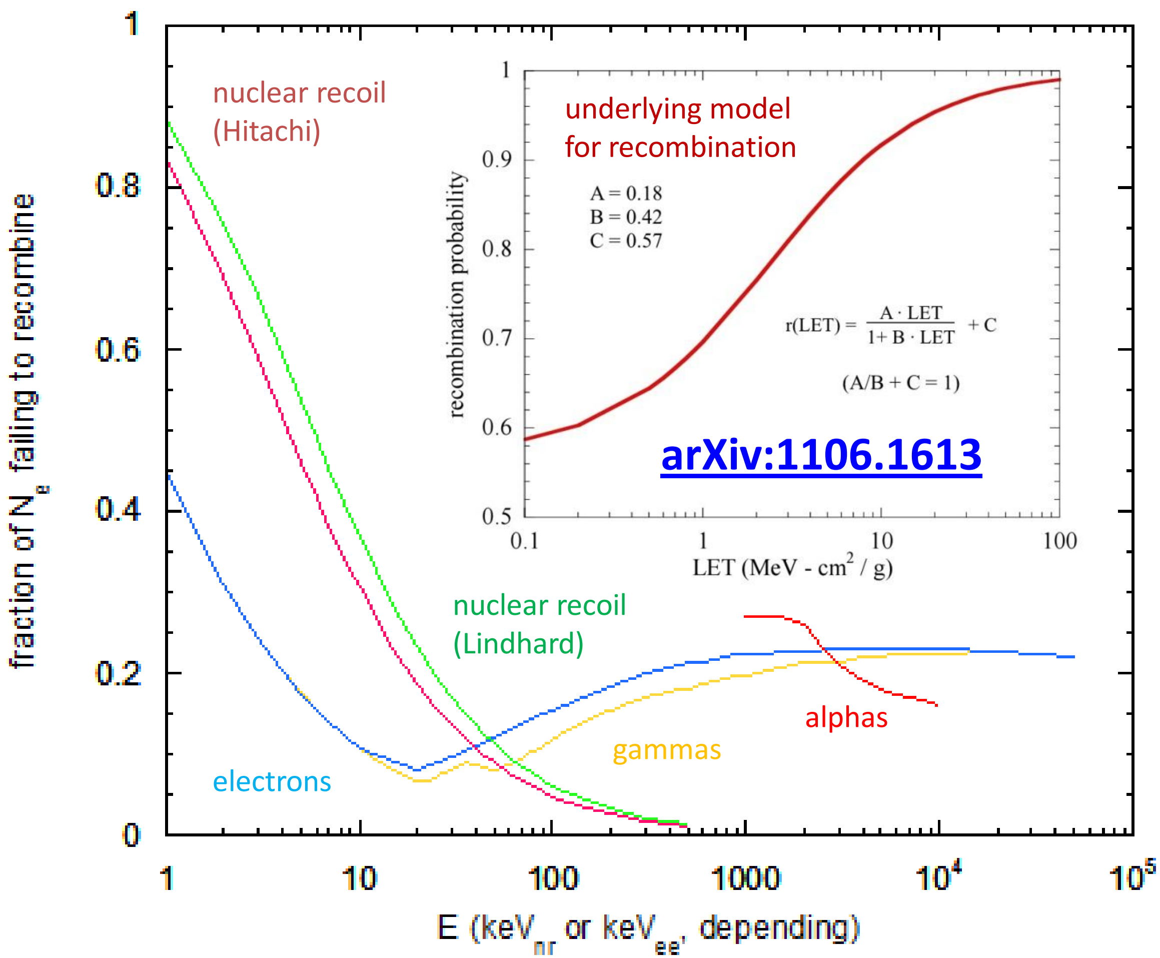


The Recombination Probability

1 – (overall recombination frac), or, the escape frac

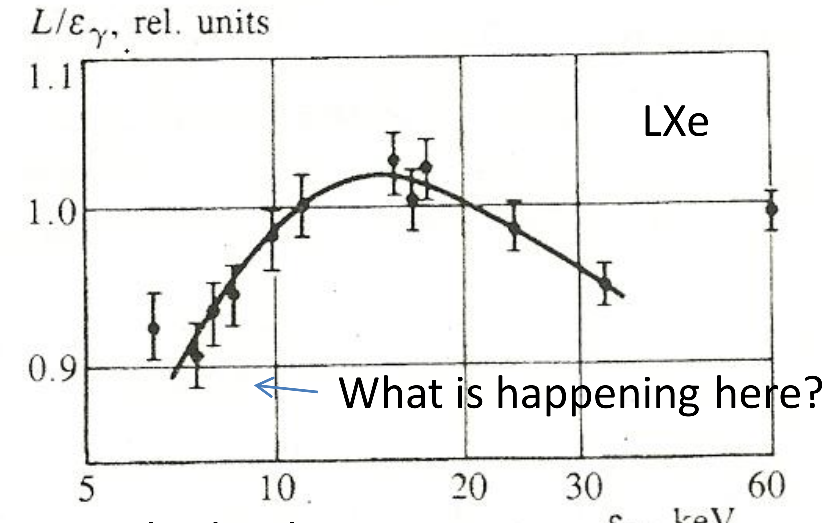


Not clear *a priori* what curve to use (at upper right) as a basis for entire model. Birks' Law of scintillation? Jaffé?

- Needed for predicting the light yield correctly (at least for LXe, LAr): most of the scintillation comes from recombined electrons (not excited)
- Many theories, models exist; we combine two physically motivated ones that fit majority of xenon data and fit best
- Curve adapted/splined continuously for electric fields: more field implies more low-energy ionization e's (from the higher-energy recoils) escape (and drift)

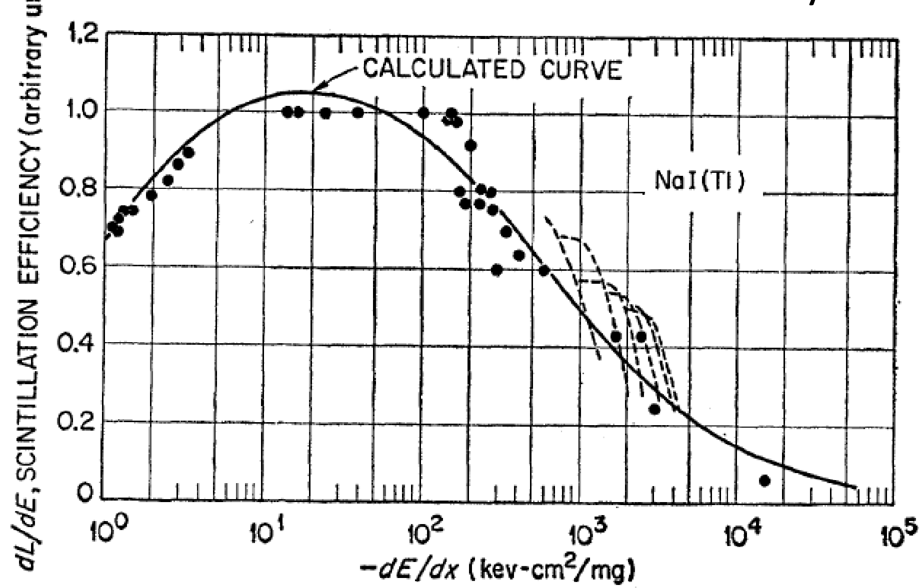
Anomalous Low-Energy Behavior

- Seen also in NaI(Tl) crystal
- Important region we must understand: what happens to electron/nuclear recoil discrimination here? What backgrounds are relevant?
- Unnatural for noble, and cannot be explained by a simple turn-over in the recombination probability
  - How to explain why a 5 keV γ scintillates less than 10?
  - Makes electron recoils look more like nuclear recoils
- Not understood until recently -- an $\mathscr{L}_{eff}$ clue…?



Obodovskii 1994

Murray 1961

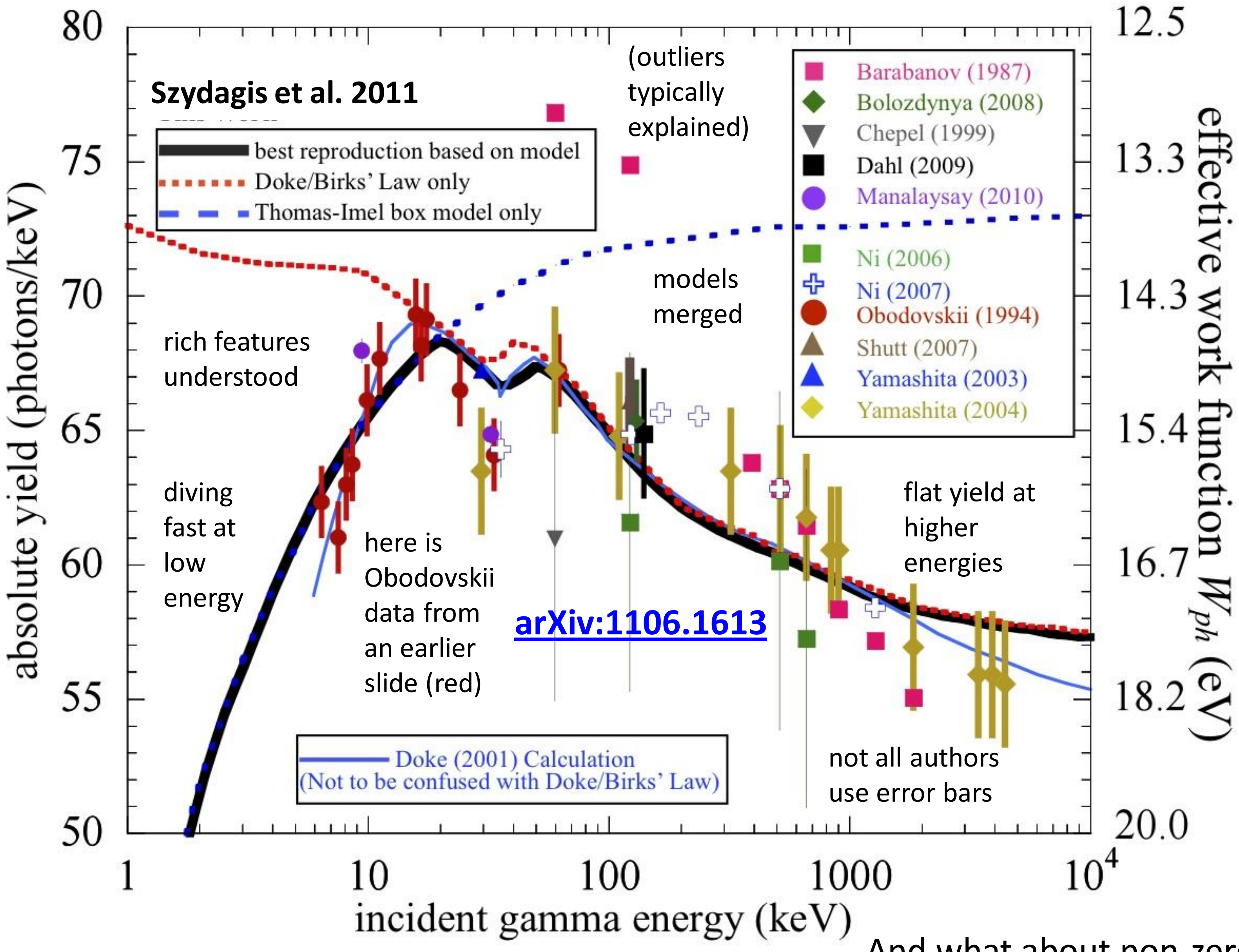


A Solution at Long Last?

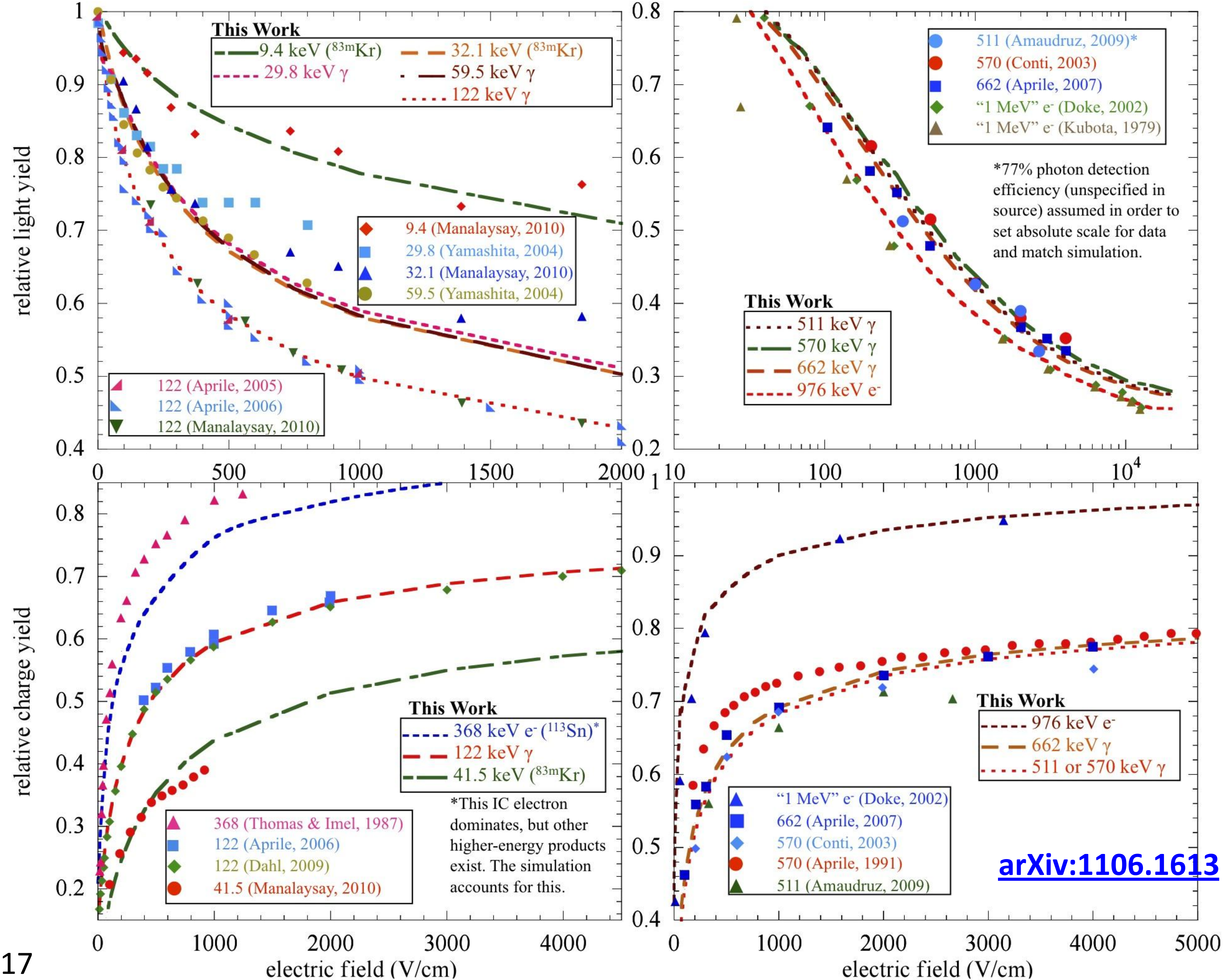
- Lower energy particles have shorter ranges (generally)
- In terms of physics we define "short range" as being smaller than the electron-ion thermalization distance: about 4-5 μm (Mozumder, 1995)
- More electrons get away without recombining and going on to make scintillation (original concept from the Ph.D. Thesis of C.E. Dahl, 2009)
- A marriage of two models: Thomas-Imel model to explain short-range particles, and Doke (modified form of Birks') for long-range: box vs. column geometries
- Same physics, but in different limits; in Thomas-Imel limit, recombination is independent of dE/dx

Putting it All Together to Predict the Yield

First: Let's look at zero-field scintillation yield from gamma rays



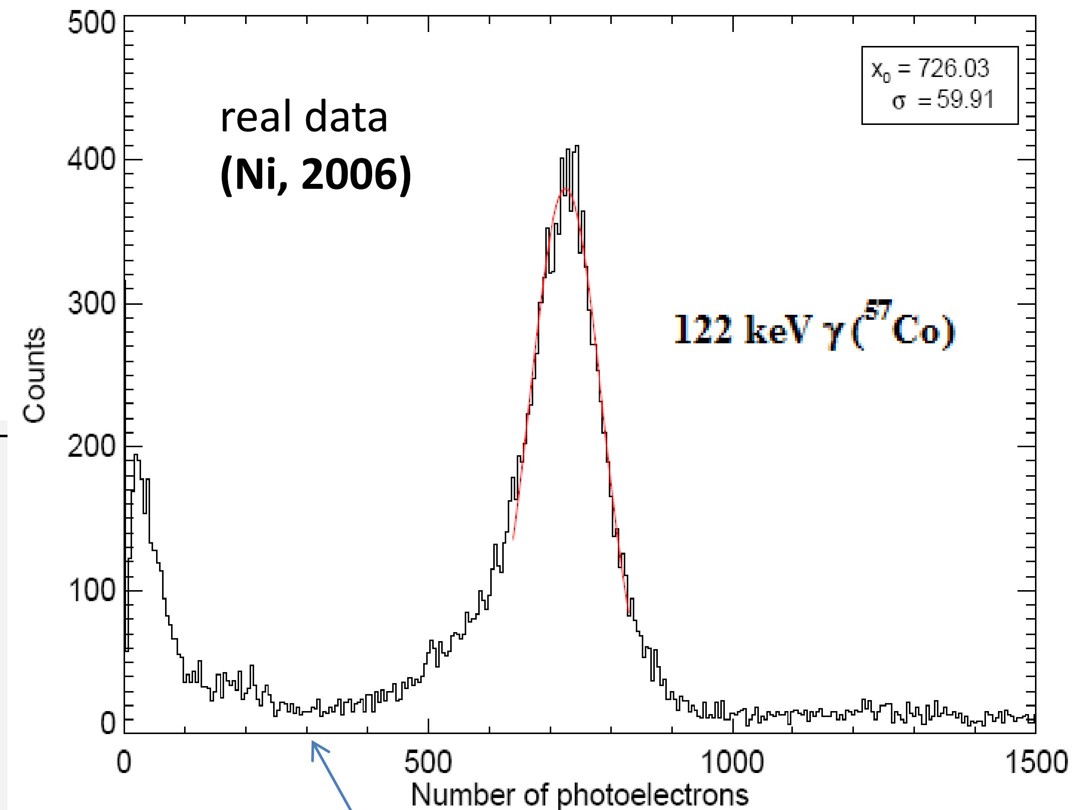
And what about non-zero field...?

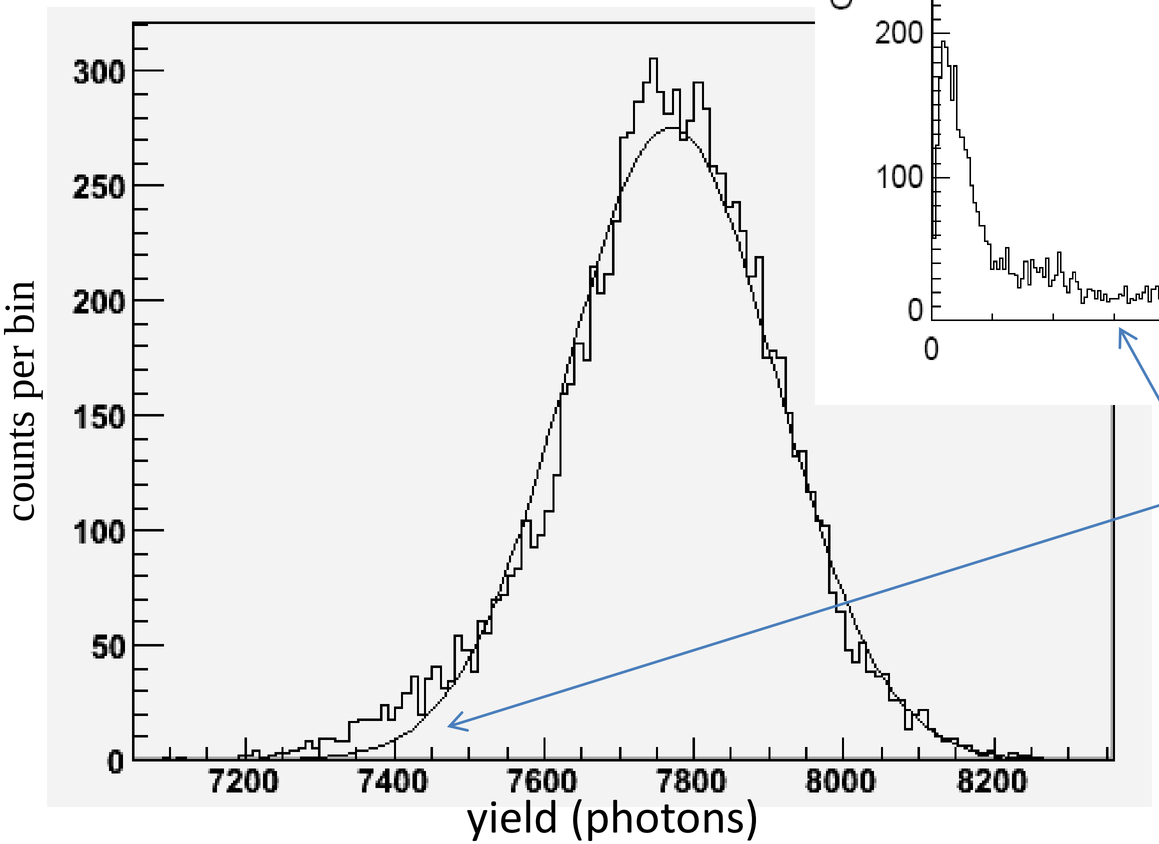


arXiv:1106.1613

Reproducing the Spread of the Yield

Geant4 toy xenon model simulation at the lower left, with the spread dominated by stochastic, individual dE/dx fluctuations along tracks

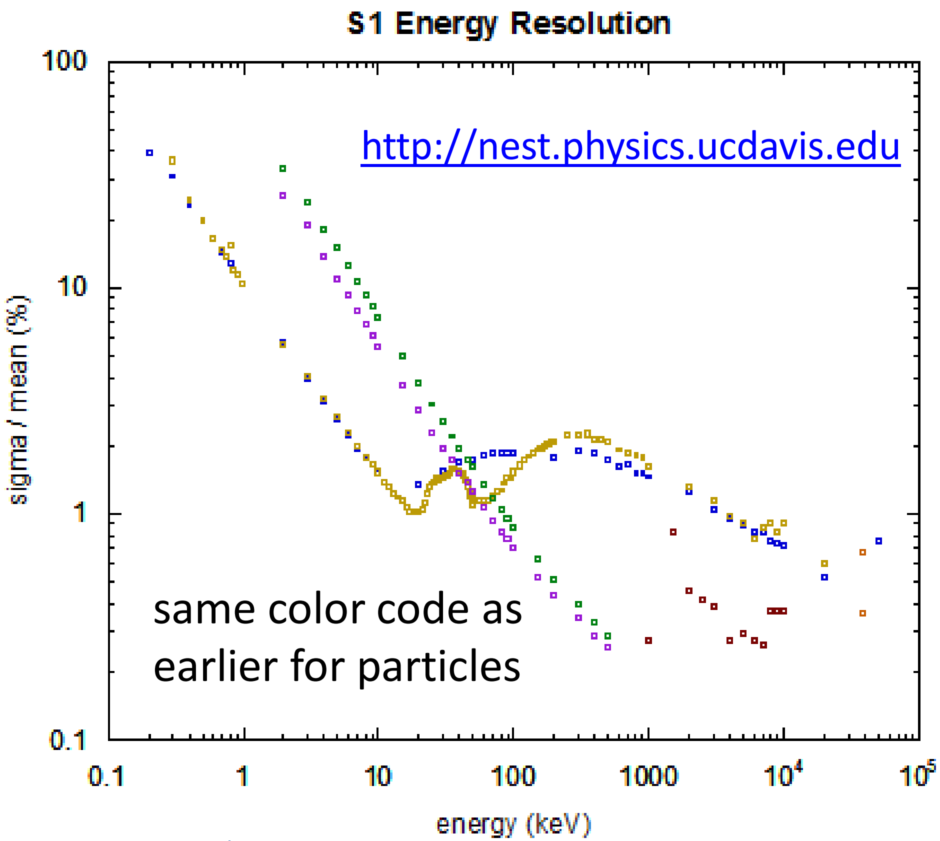


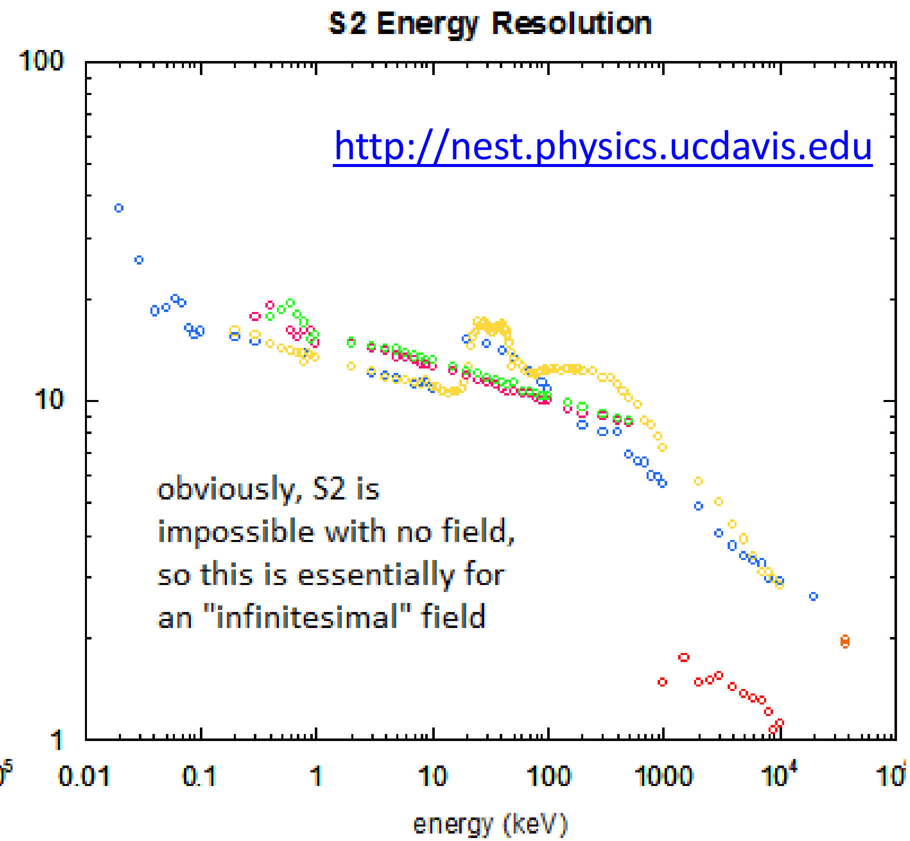


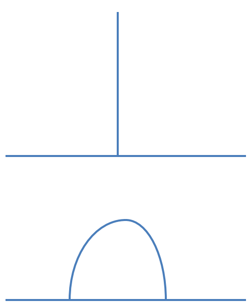
similar asymmetrical shapes, caused a bit by characteristic x-rays indirectly produced by one parent gamma, and by detector effects

Energy Resolution

Preliminary NEST Predictions for Zero Electric Field



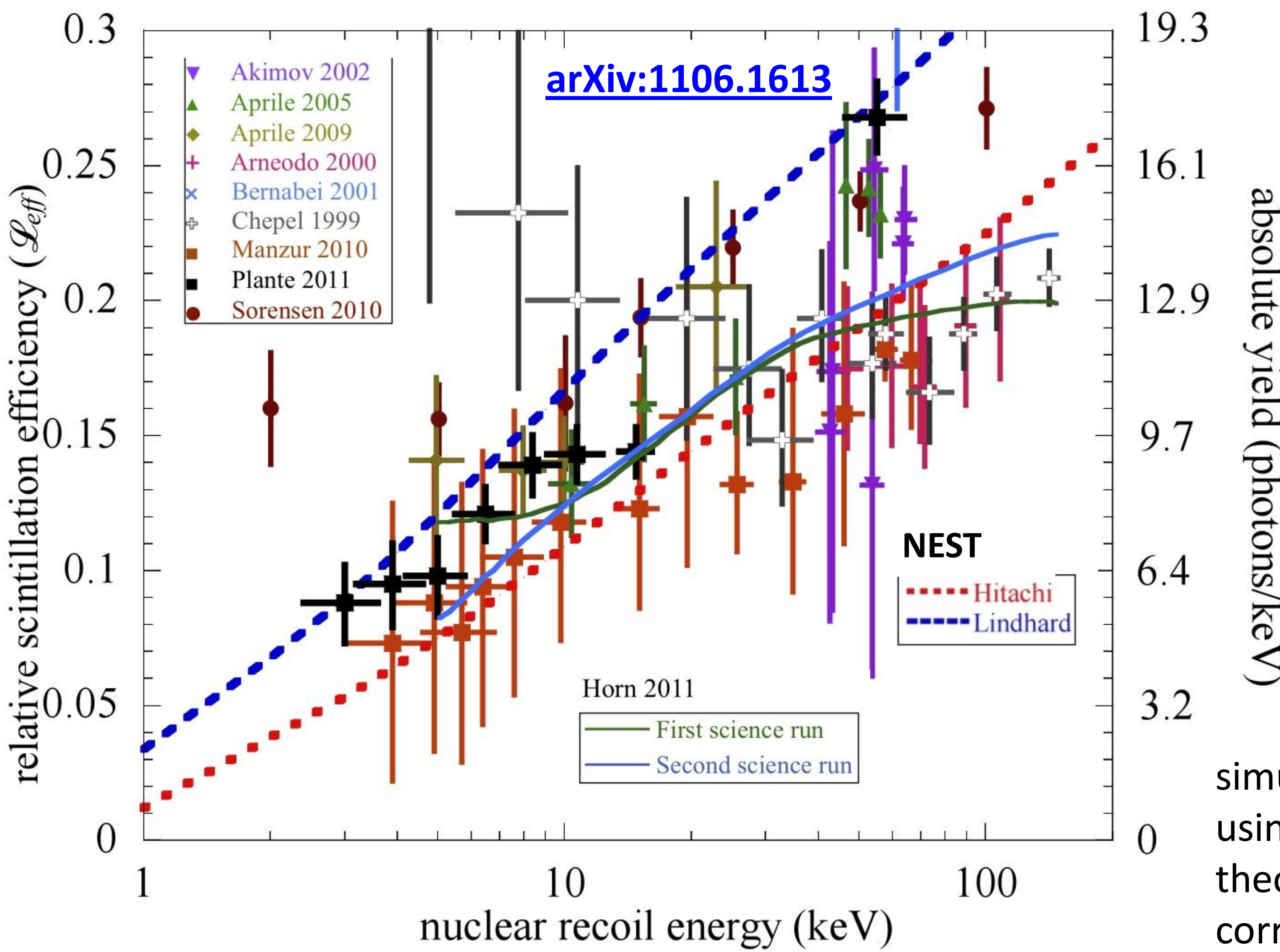




The sources of INTRINSIC non-perfect resolution, at all electric fields

- Fano factor (extremely small effect until lower energies)
- Binomial fluctuations in the recombination probability
- Binomial fluctuations in the numbers of excitons versus ions (small)
- Particle track history, including stochastic dE/dx effects

Switching Gears: Nuclear Recoil



prediction with simulations based on electron recoil numbers, NOT a direct fit

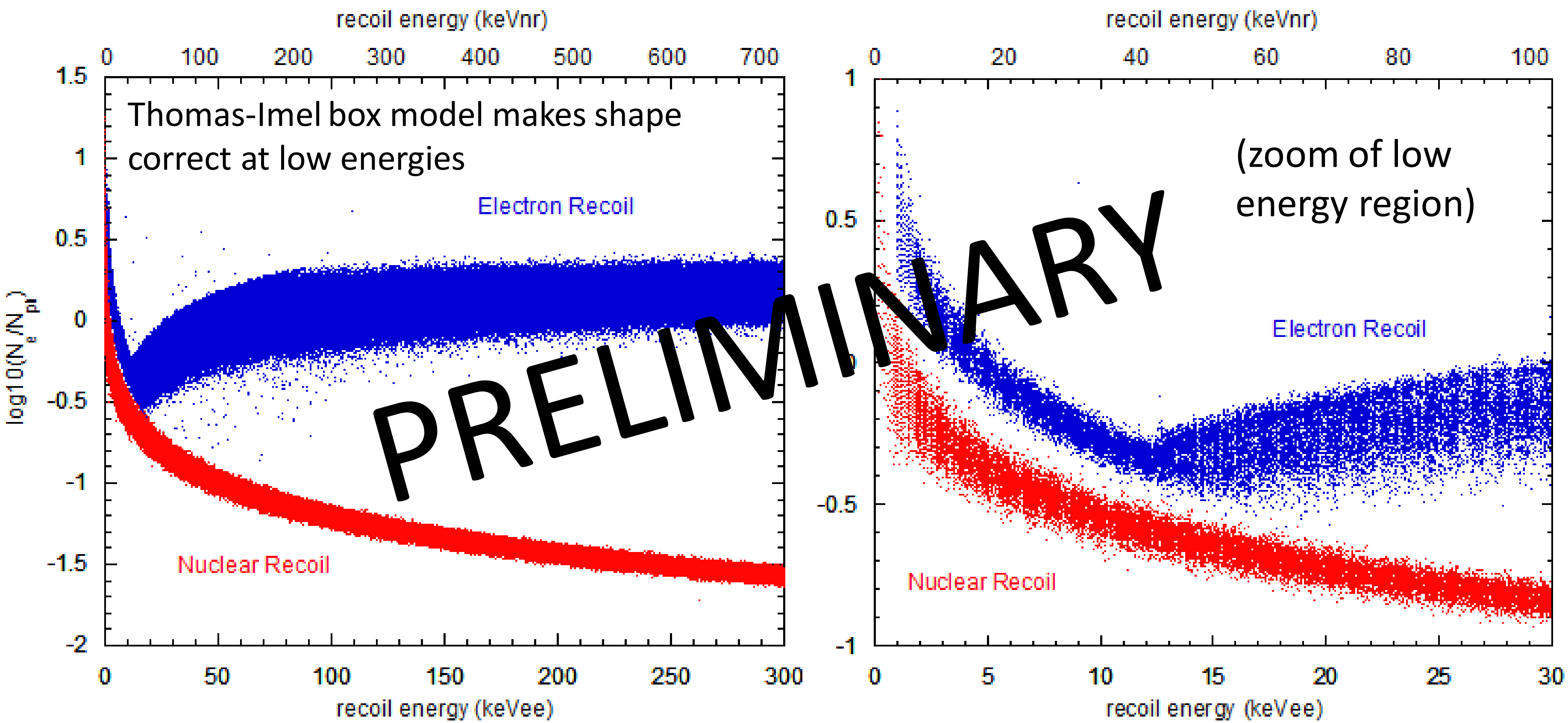
(other axis is relative to 122 keV gamma's yield, as is traditional)

simulated yield using Lindhard theory or the Hitachi correction to it

This is likely the strongest prediction, with the simplest assumptions, ever devised!

Simulated ER and NR bands in S2/S1

0.45 kV/cm electric field

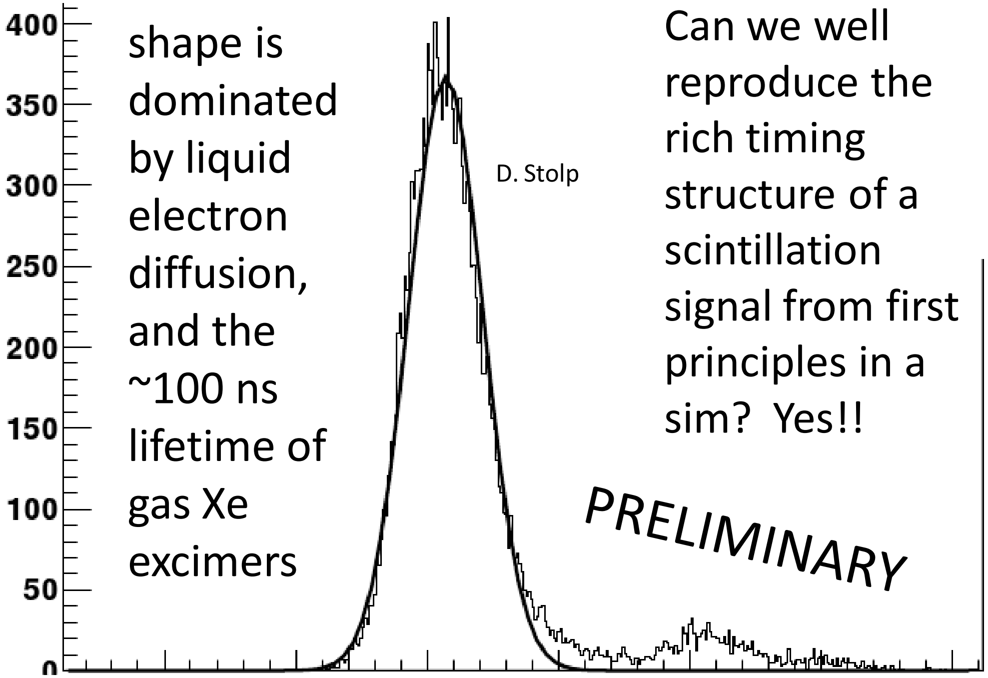


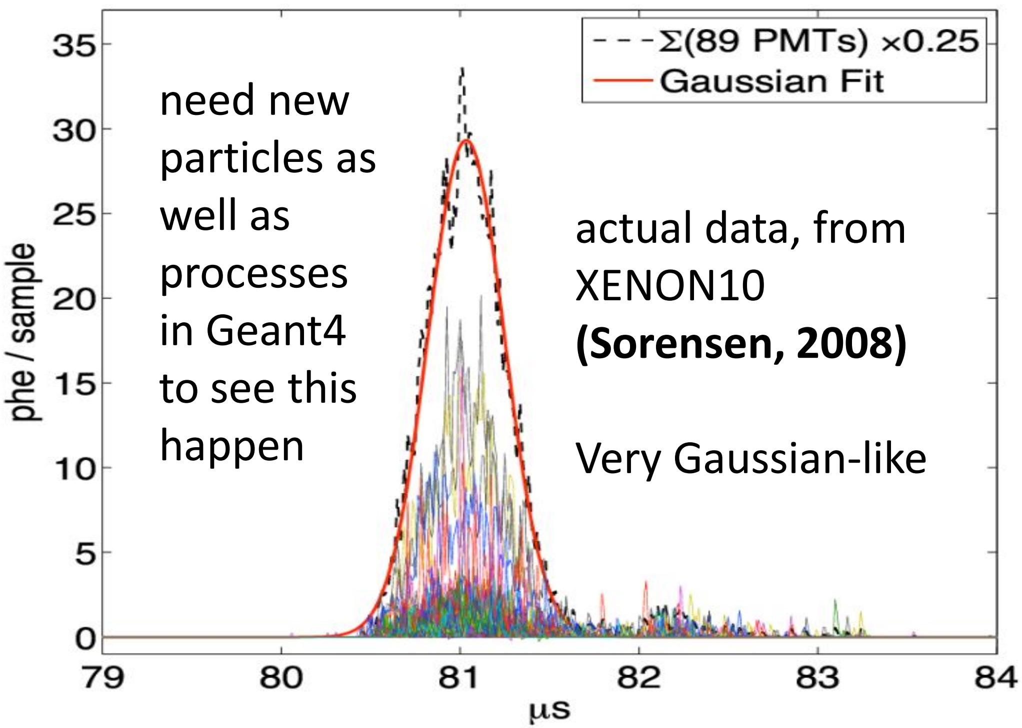
NO artificial smearing, Gaussian or otherwise, was added to NEST to yield the result depicted.

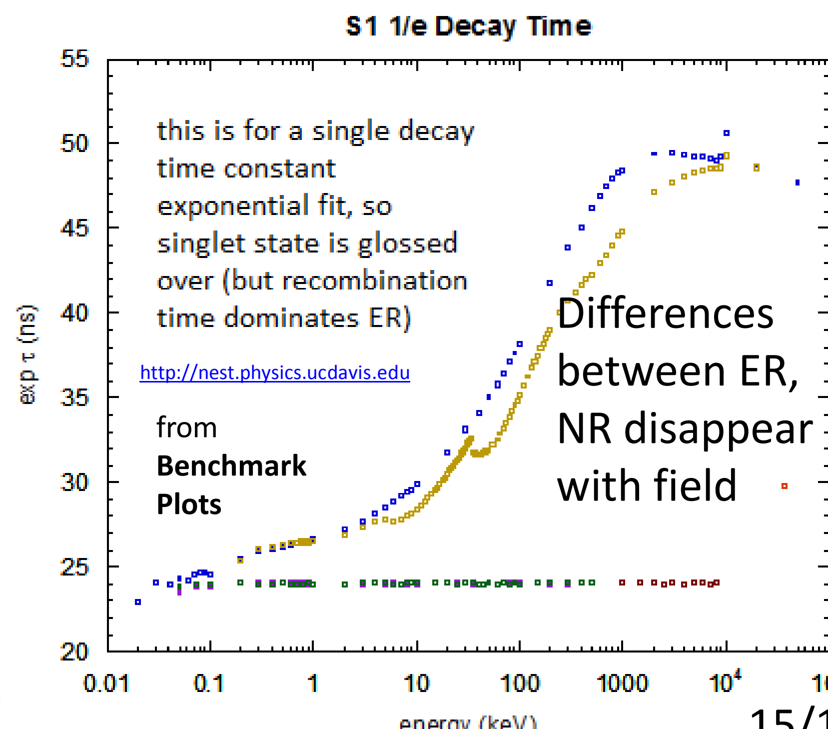
Now it has become possible, with NEST, to study/predict the discrimination power of your experiment before you even built it or calibrate, with a reliable simulation.

Understanding the Raw Pulse Shapes (S1, S2)

single, triplet lifetimes incorporated for S1, as well as the recombination time, which is varied versus ionization density and the electric field magnitude







LXe Properties: The Finer Points

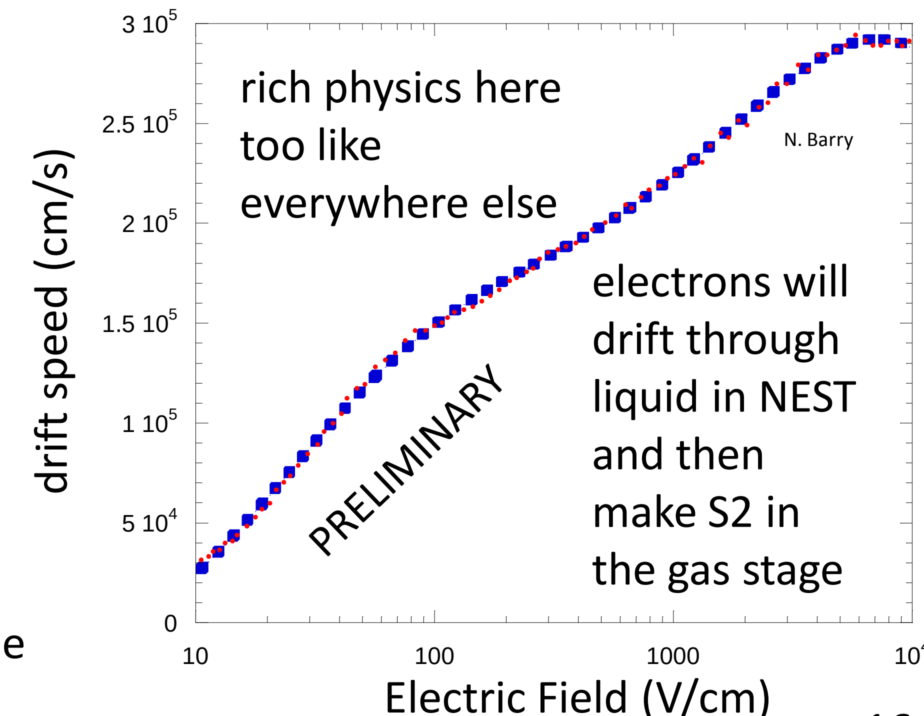
- We compiled all available (Xe) experimental data in the literature and performed a meta-analysis of it
- NEST scintillation wavelength is 178 nm (6.97 eV) with 14 nm FWHM, consistent with past results
- Compiled lifetimes, ratios for singlet, triplet states (unique for the different interaction types!)
- Studied physics of electron drift, so we can soon more fully simulate 2-phase detectors with NEST in Geant4

Particle	τ_1	τ_3	A_1/A_3
e	2.2 ± 0.3	27 ± 1	0.6 ± 0.2
α	$3.77 \pm 0.31^{*}$	$23.7 \pm 2.4^{*}$	$11.6 \pm 9.71^{*}$
$n{+}^{252}\mathrm{Cf}$	5.1 ± 0.45	23.2 ± 1.5	7.8 ± 1.5

N. Walsh

liquid xenon thermal electron drift velocity versus electric field (data in red, fit in blue)

Will tell you your drift time



Status and Future

- Upgrade to **G4Scintillation** physics process, called **G4S1Light**, available for download on-line; speaking with GEANT about inclusion in upcoming version
- Fully simulating DAQ chain (pulse shaping, etc.)
- Another new G4 physics process: **G4S2Light** soon!
- Representatives of many collaborations already members of the NEST mailing list, and downloading
- No more rules of thumb, nor extrapolations from past detectors: build your geometry and go
- Dial in a particle type and energy, set your electric field, and watch your sims give reliable results
- Next: GXe, L/GAr, Ne, He, Kr, solids – complete?

References

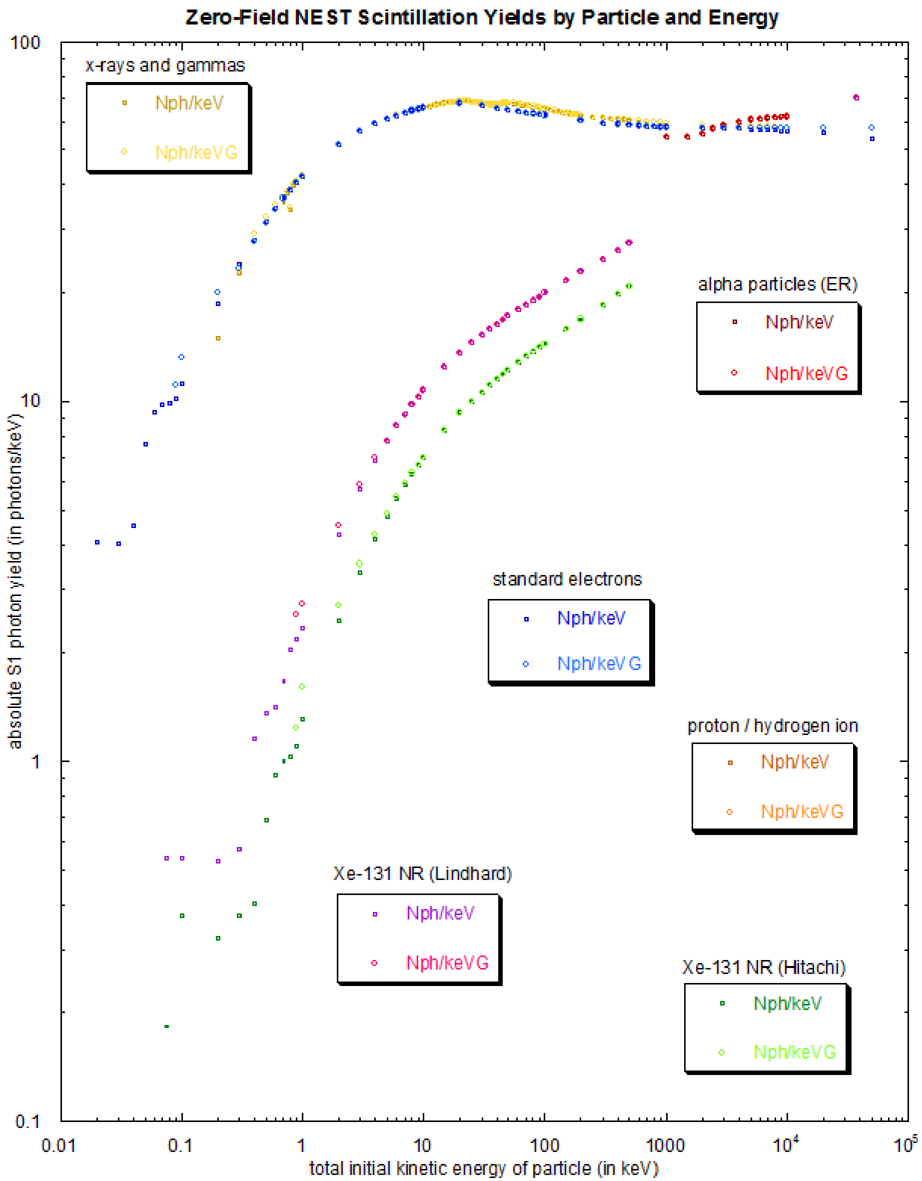
- For all of the references used in this talk, please simply consult the full bibliography of

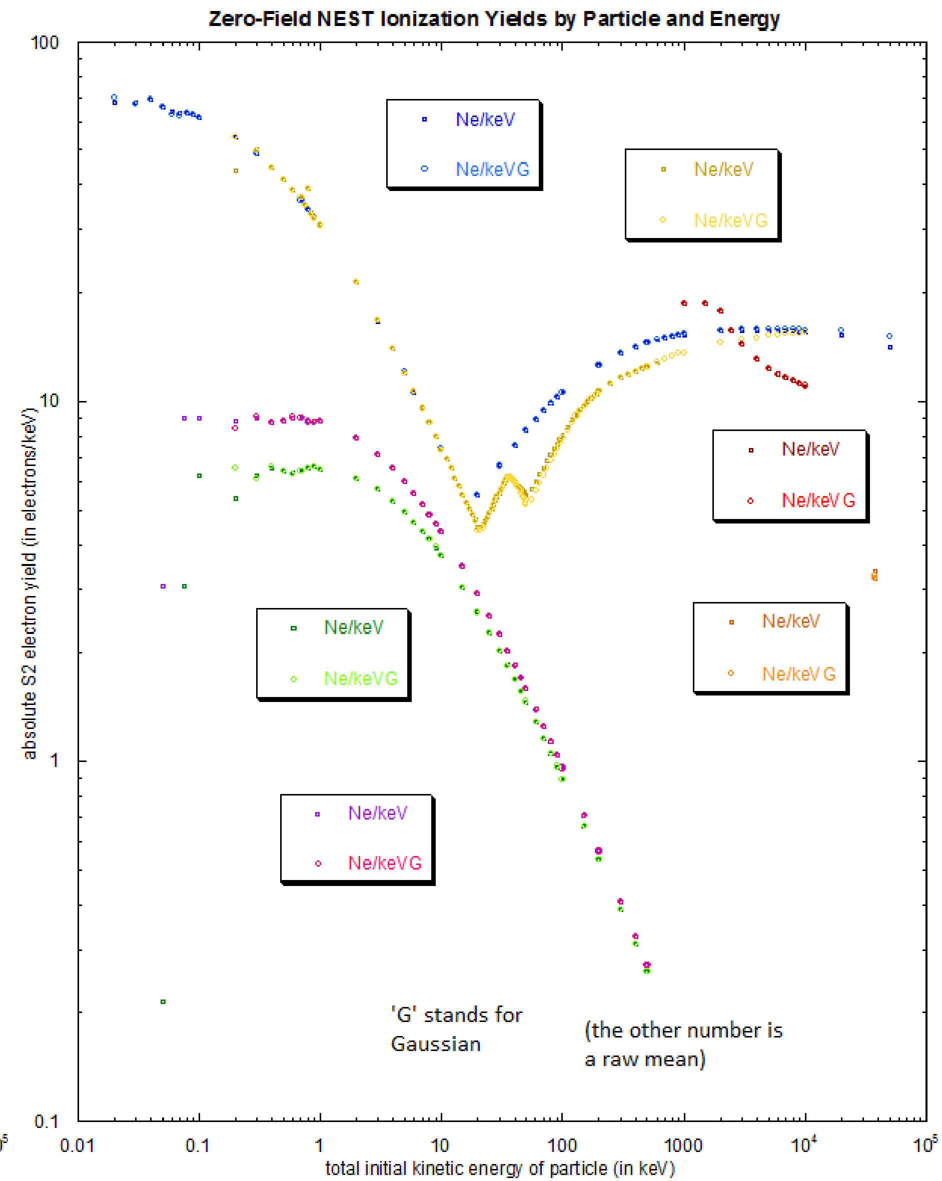
Szydagis et al., NEST: A Comprehensive Model for Scintillation Yield in Liquid Xenon, arxiv:1106.1613, June 2011. Submitted to JINST, and accepted for publication, September 2011, in press.

謝謝

THANK YOU

Bonus Slides





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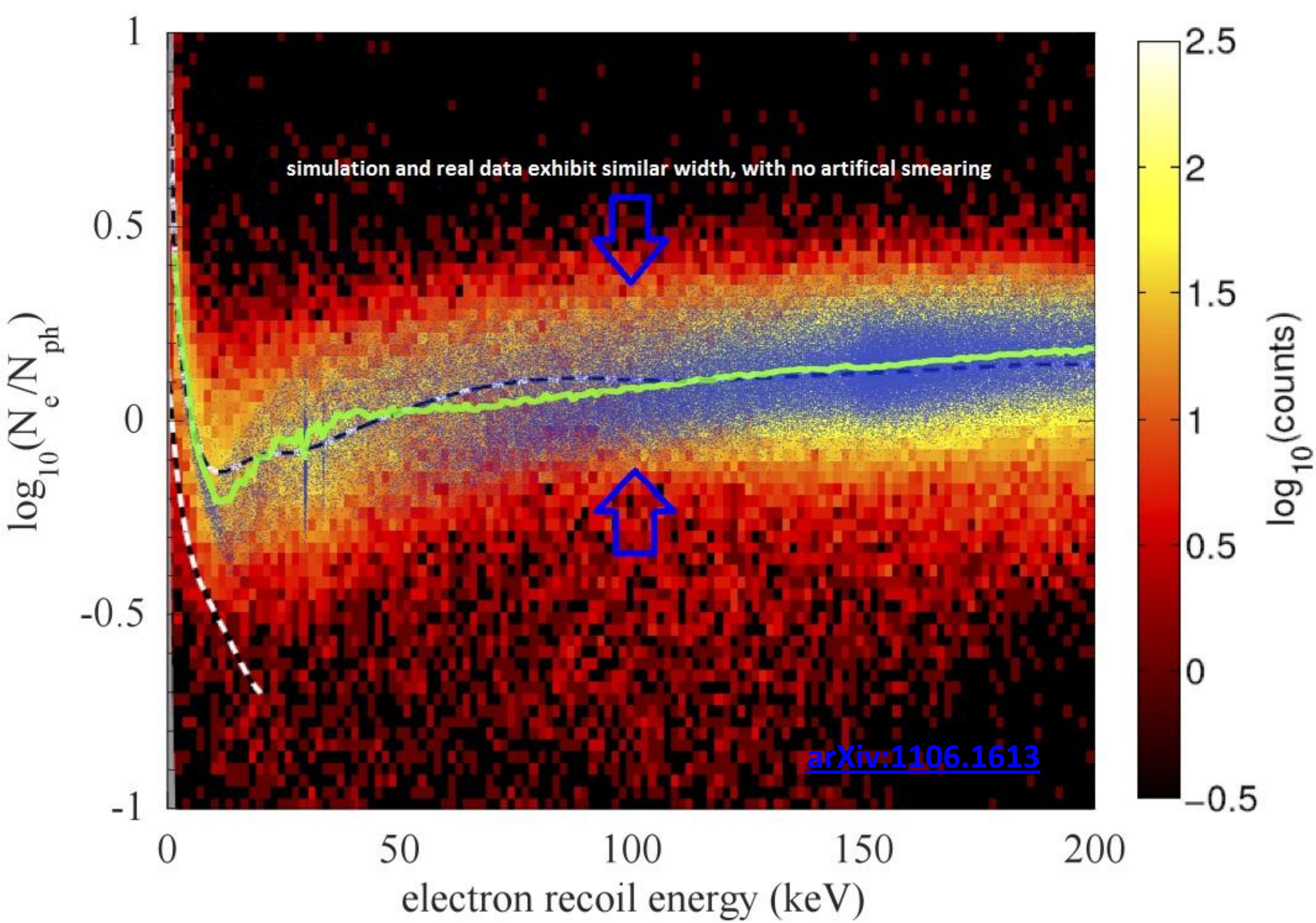
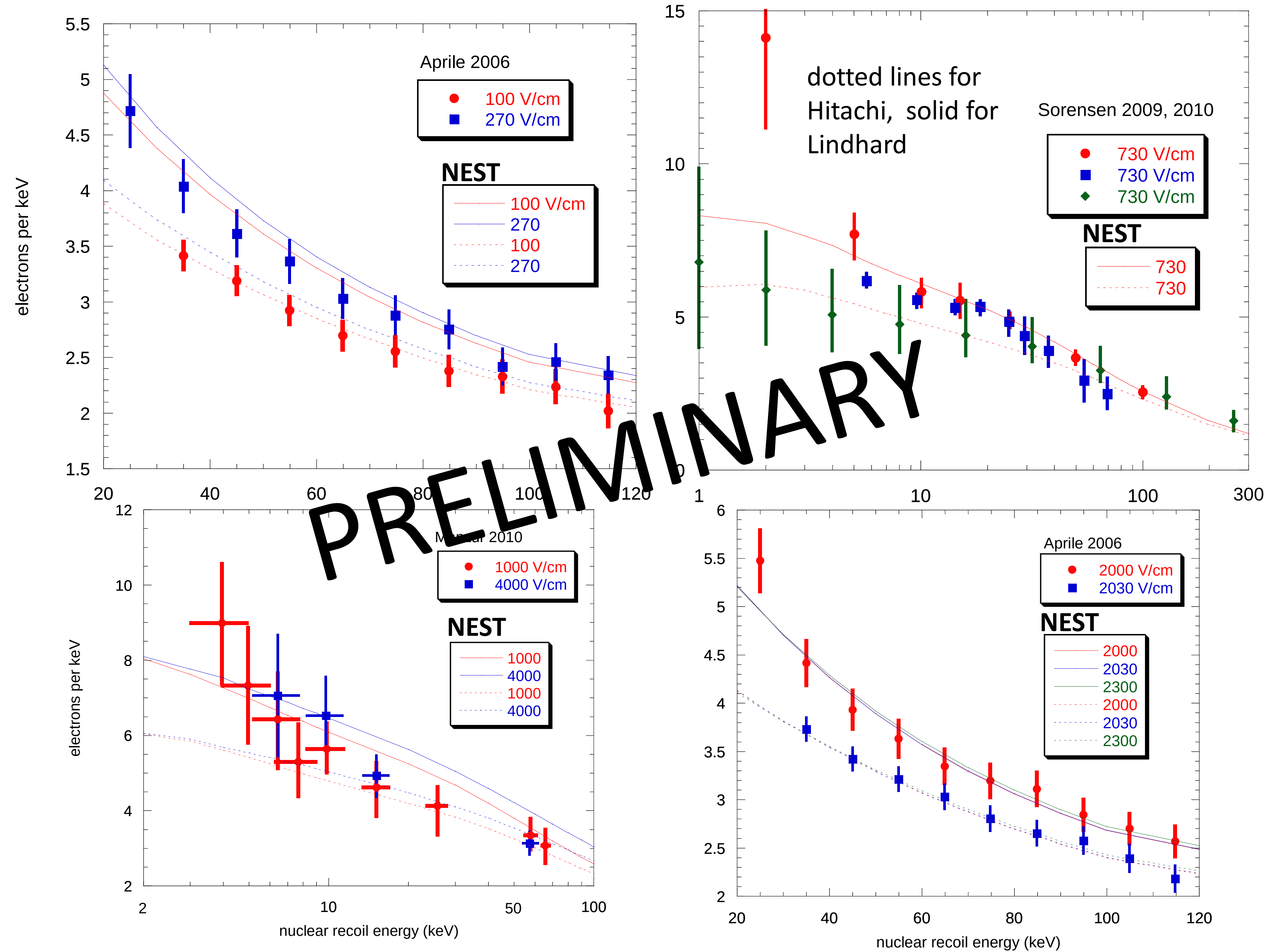
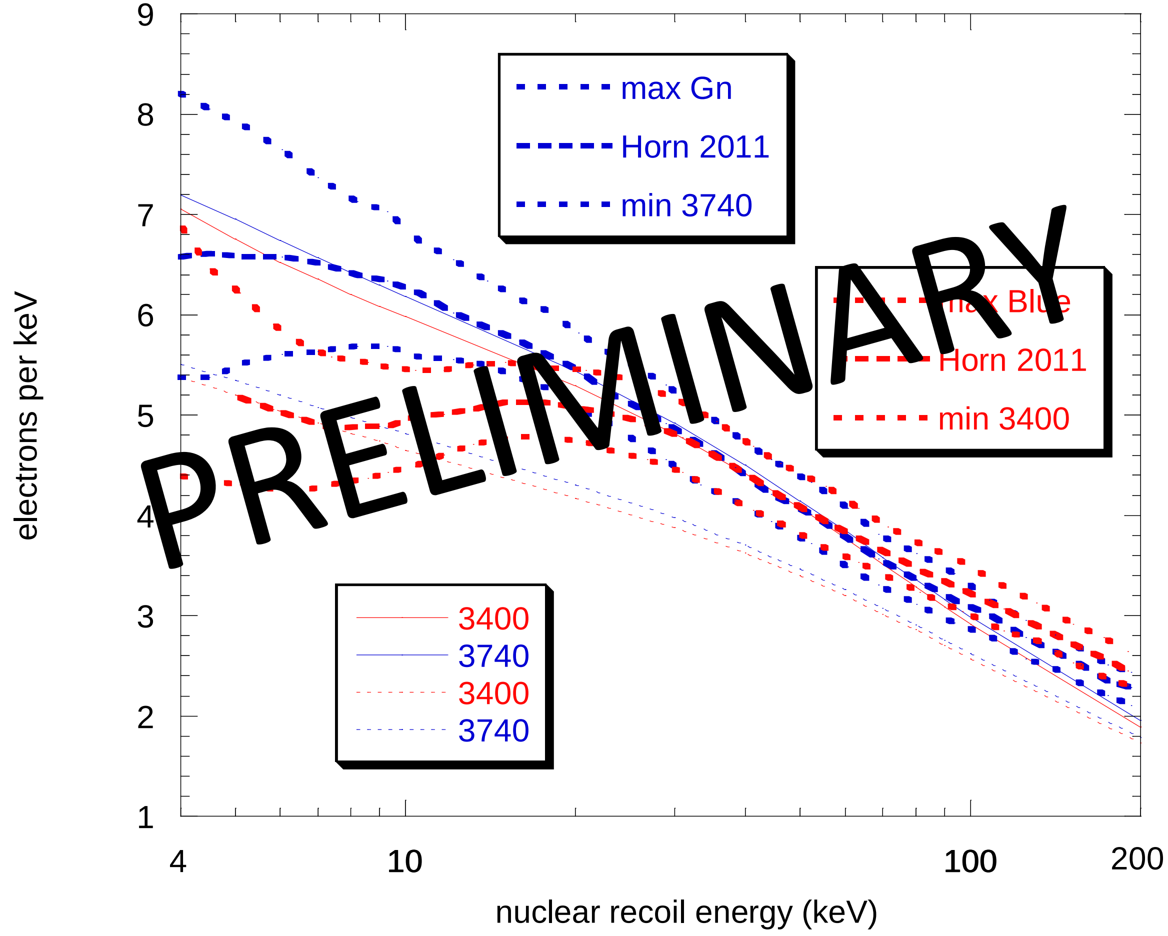

simulation and real data exhibit similar width, with no artifical smearing
arXiv:1106.1613
log10(Ne/Nph)
electron recoil energy (keV)
log10(counts)
1
0.5
0
-0.5
-1
0
50
100
150
200
2.5
2
1.5
1
0.5
0
−0.5


PRELIMINARY
electrons per keV
Aprile 2006
100 V/cm
270 V/cm
NEST
100 V/cm
270
100
270
dotted lines for Hitachi, solid for Lindhard
Sorensen 2009, 2010
730 V/cm
730 V/cm
730 V/cm
NEST
730
730
2010
1000 V/cm
4000 V/cm
NEST
1000
4000
1000
4000
electrons per keV
nuclear recoil energy (keV)
Aprile 2006
2000 V/cm
2030 V/cm
NEST
2000
2030
2300
2000
2030
2300
nuclear recoil energy (keV)



max Gn
Horn 2011
min 3740
max Blue
Horn 2011
min 3400
3400
3740
3400
3740
PRELIMINARY
electrons per keV
nuclear recoil energy (keV)
9
8
7
6
5
4
3
2
1
4
10
100
200