Improving Scintillation Response in Xenon and Implementation in GEANT4

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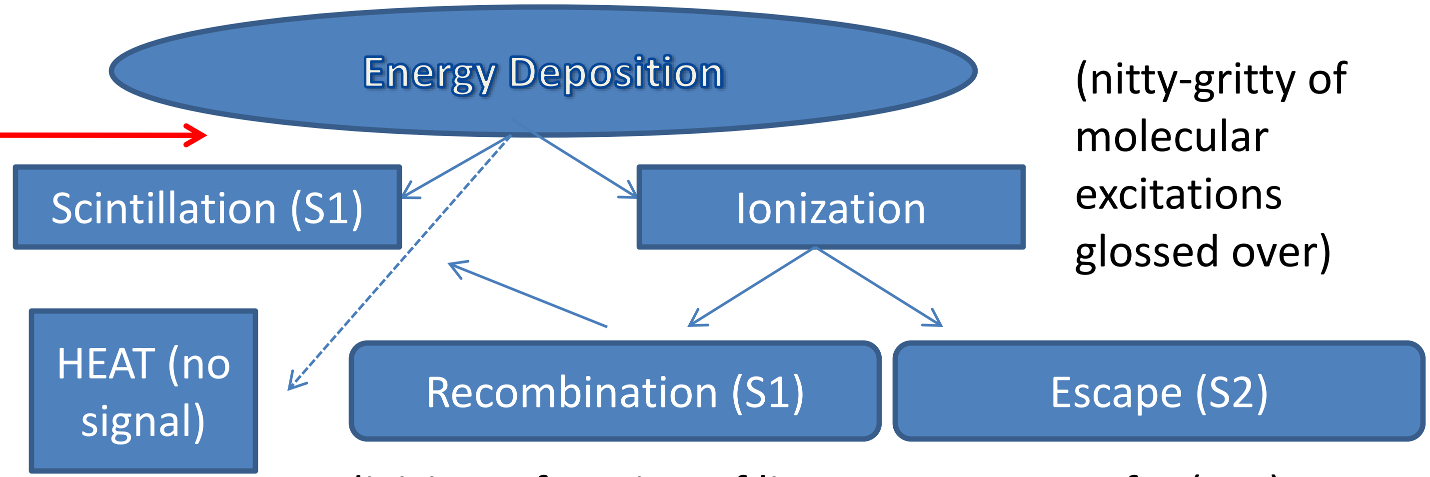
Purpose

- Create a full-fledged simulation based on a heuristic, quasi-empirical approach
- Comb the wealth of data for liquid and gaseous noble elements for different particles, energies, and electric fields, then combine everything
- Aid the many dark matter and $0\nu\beta\beta$ decay experiments which utilize this technology to be on the same page for simulations
- Bring added realism to the simplistic model in GEANT4 present now (v4.9.4) for nobles
- Explore backgrounds at low energy by expanding GEANT4 physics to be more accurate when you go to a low energy regime: $O(1)$ keV

Basic Physics Principles

division of deposition energy 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



(nitty-gritty of molecular excitations glossed over)

(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 electric field magnitude

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

Model Framework: Electron Recoils

- Looking at the GEANT tracking verbosity: different energy depositions from the secondary electrons and gammas in an EM-cascade
- Let's allow the recombination to fluctuate stochastically by treating every electron recoil on its own

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* 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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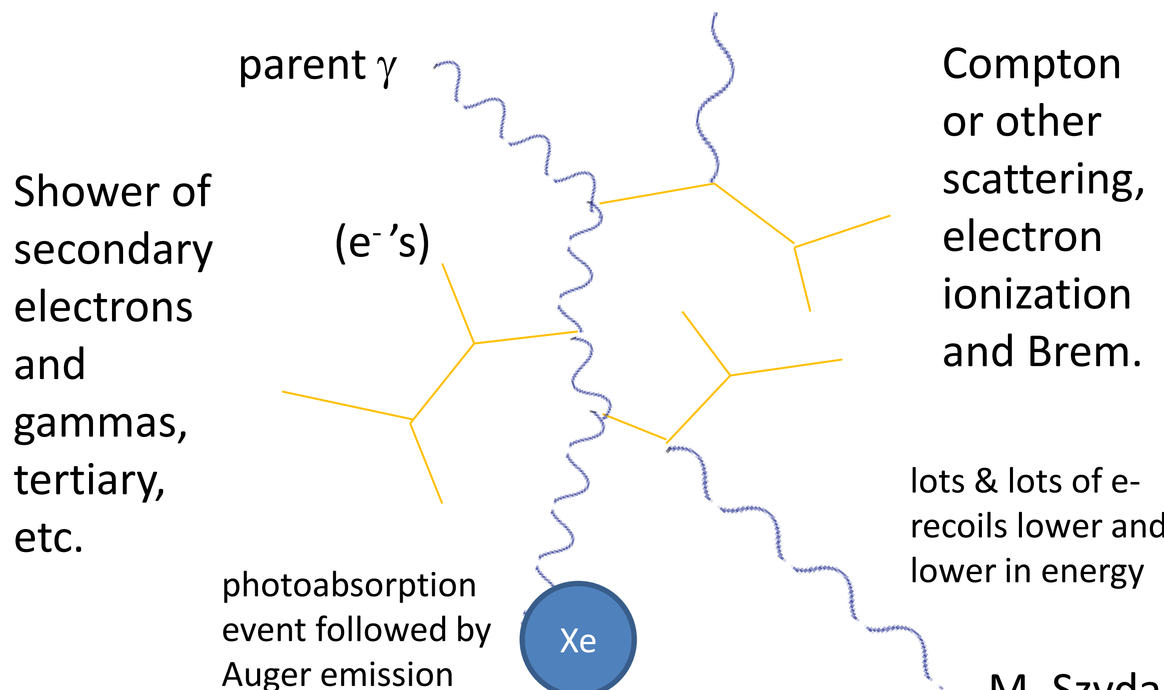
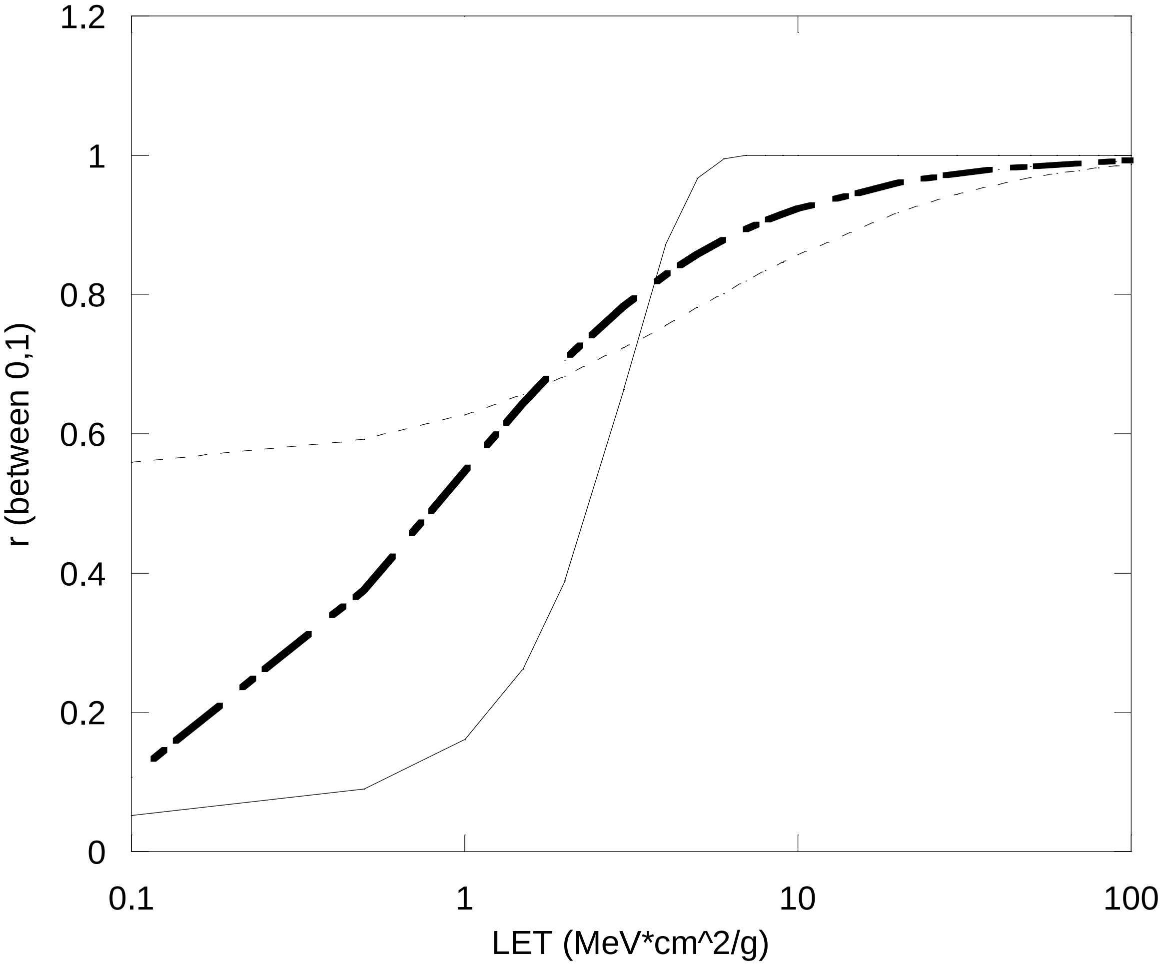


The Recombination Probability

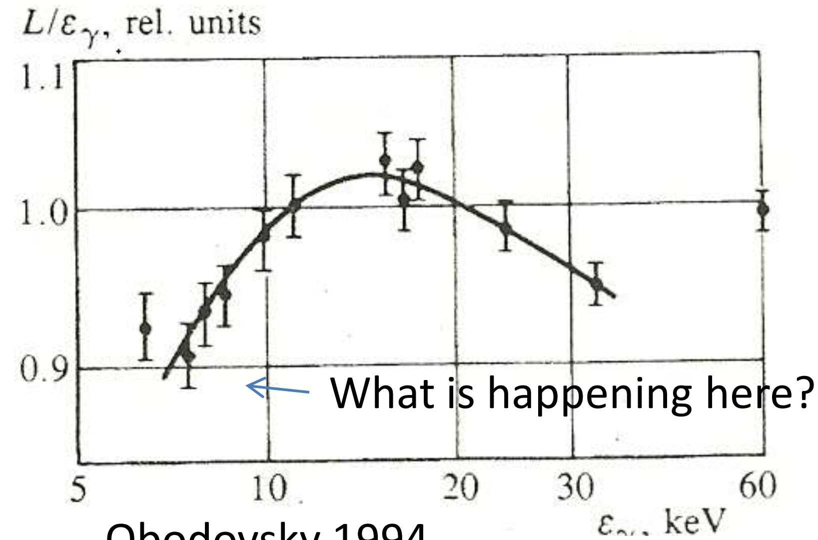


Not clear *a priori* what curve to use. Birk's Law? Jaffe?

- Important for predicting the light yield correctly (at least for Xe, Ar): most primary scintillation comes from recombined electrons (not direct)
- Many theoretical models tried; we combine theoretically 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)

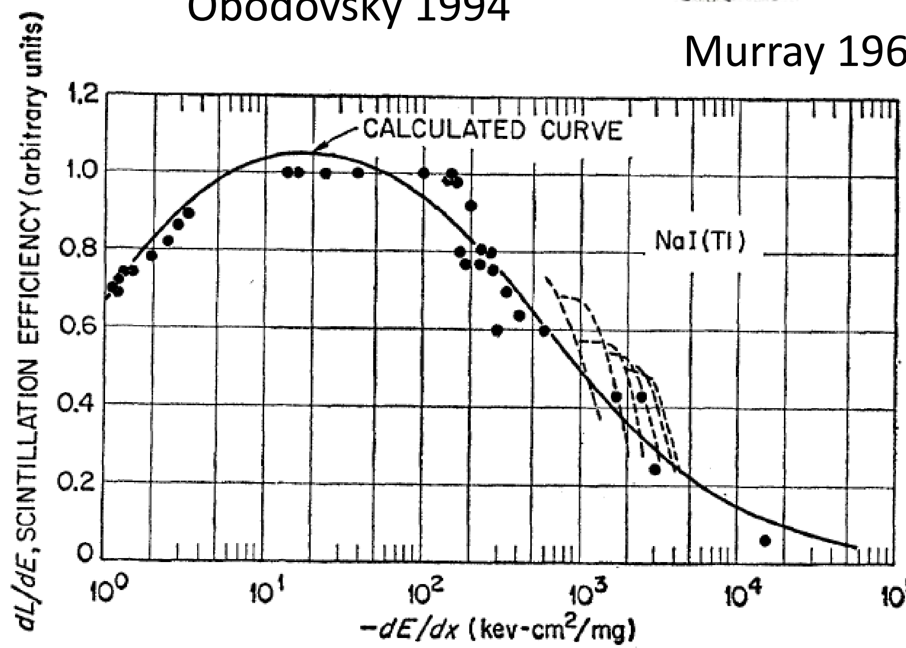
Anomalous Low-Energy Behavior

- 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 - is an $\mathscr{L}_{eff}$ clue…?



Obodovsky 1994

Murray 1961



A Solution at Last?

- Lower energy particles have shorter ranges (generally)
- In terms of physics we define "short range" as being less than the electron-ion thermalization distance of ~4.6 μm (Mozumder, 1995)
- More electrons get away without recombining and going on to make scintillation (original concept from Ph.D. Thesis of C.E. Dahl, 2009)
- A marriage of two models: Thomas-Imel box model to explain short-range particles, and Jaffe (modified Birk's) for long-range: box vs. column geometries
- Same physics, but different limits. In Thomas-Imel limit recombination is independent of dE/dx

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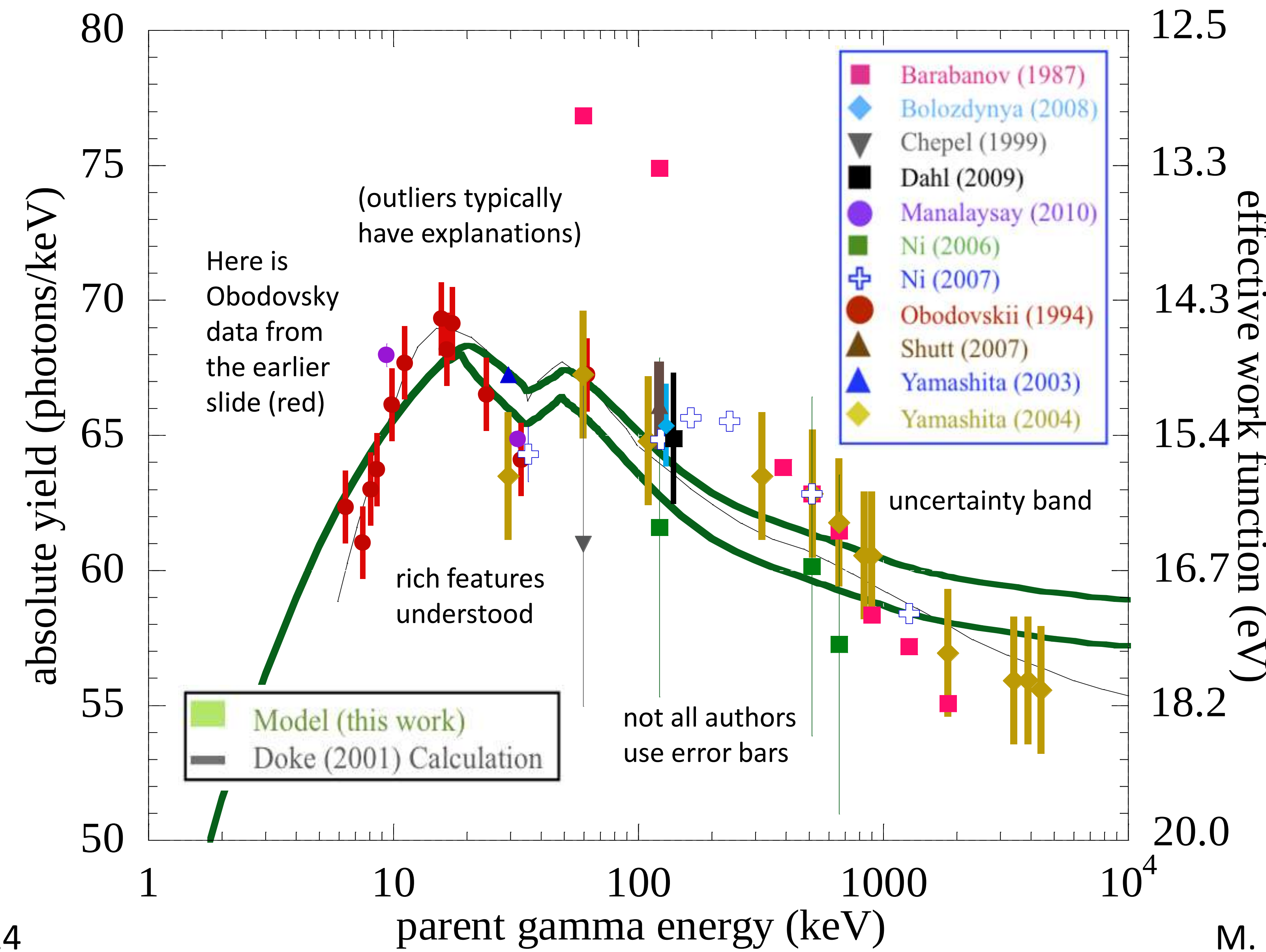
Putting it All Together to Predict Yield



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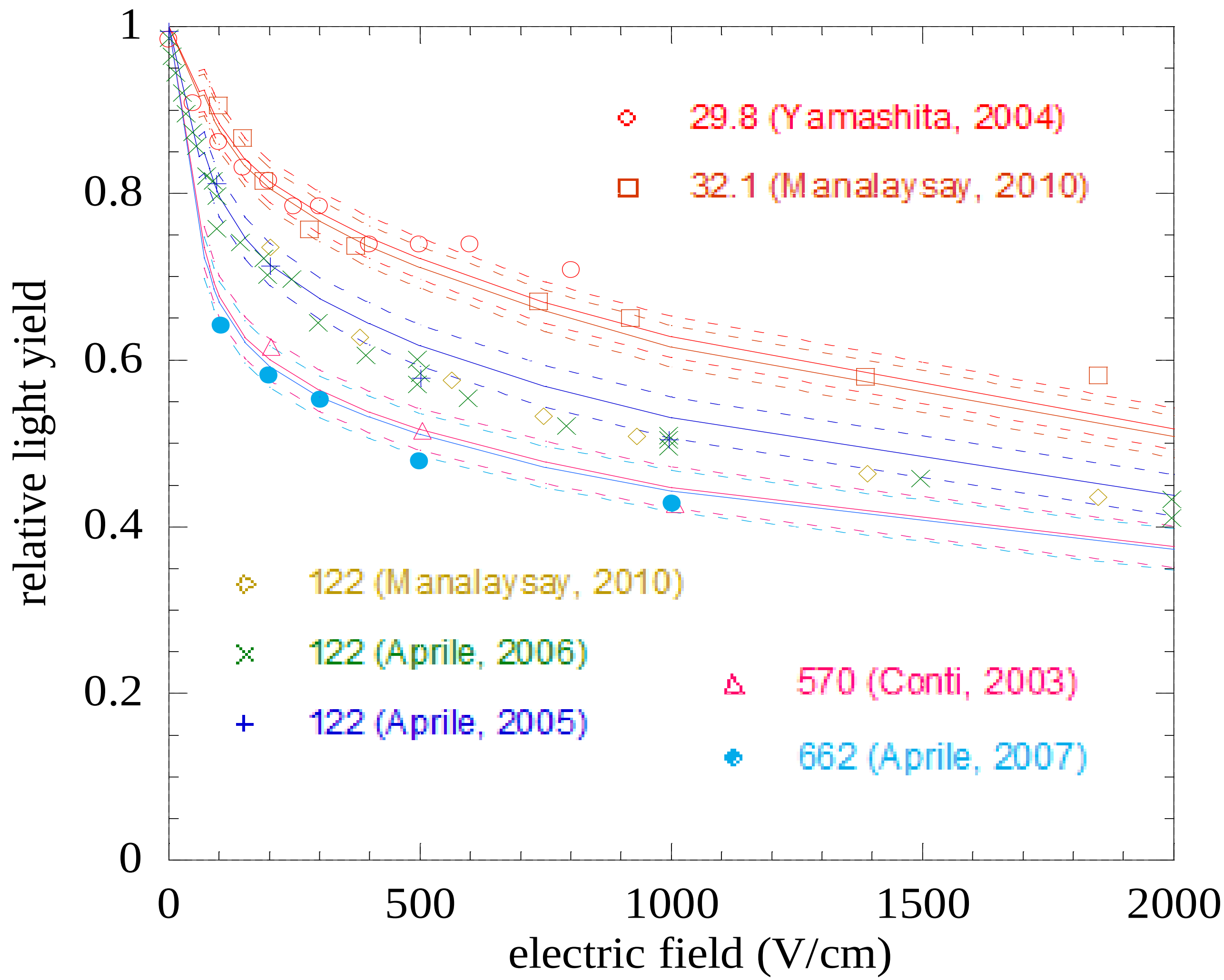
The Electric Field Dependence of Scintillation and Charge Yields



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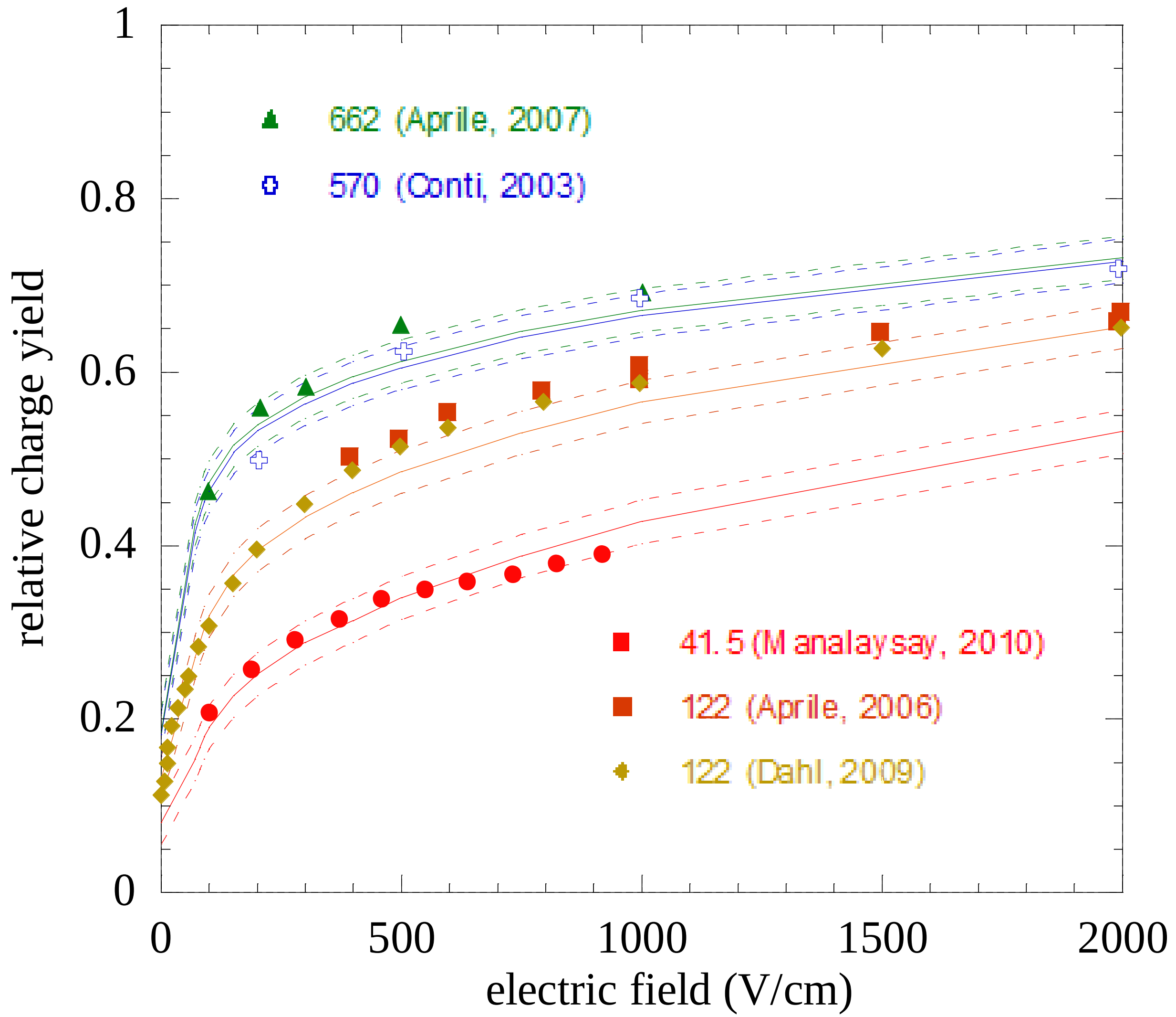
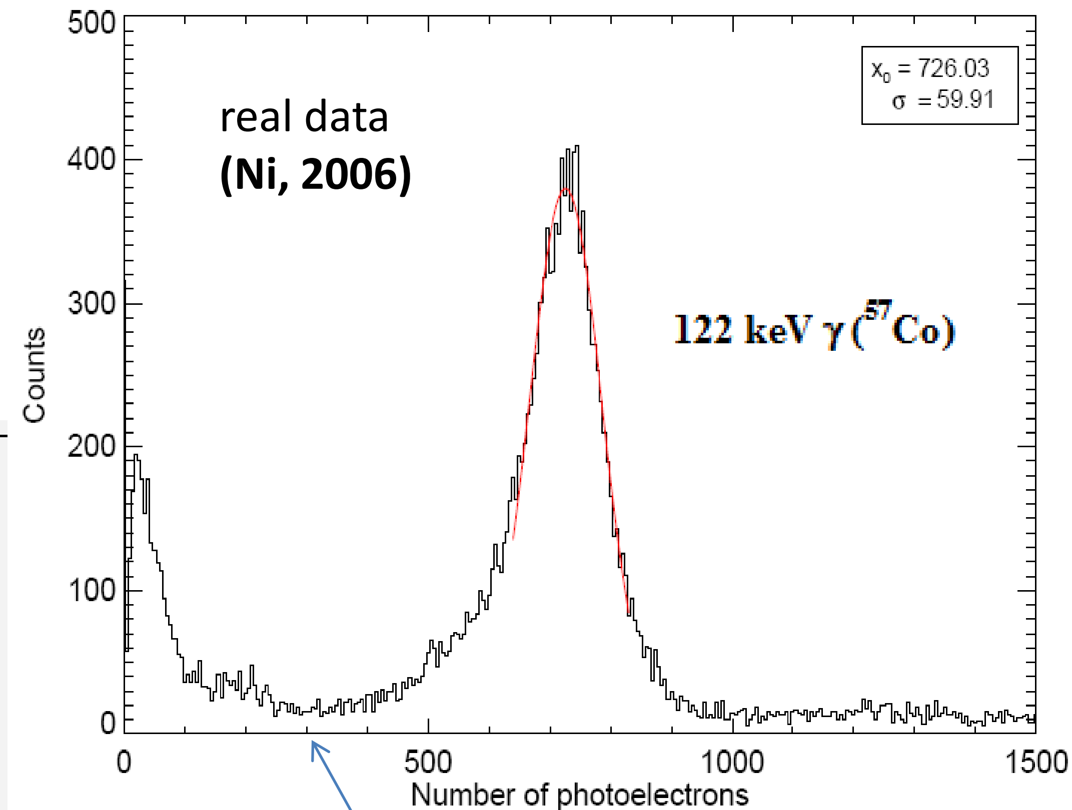
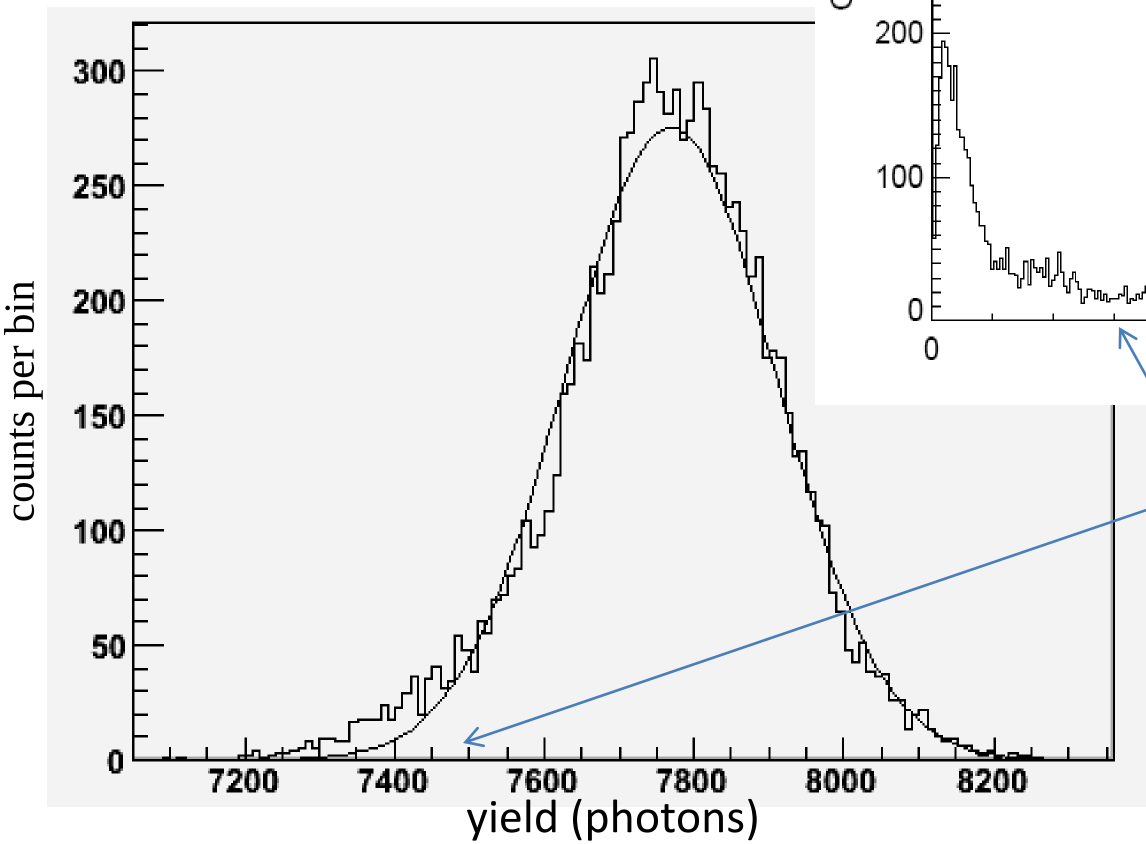


Reproducing Spread in Yield

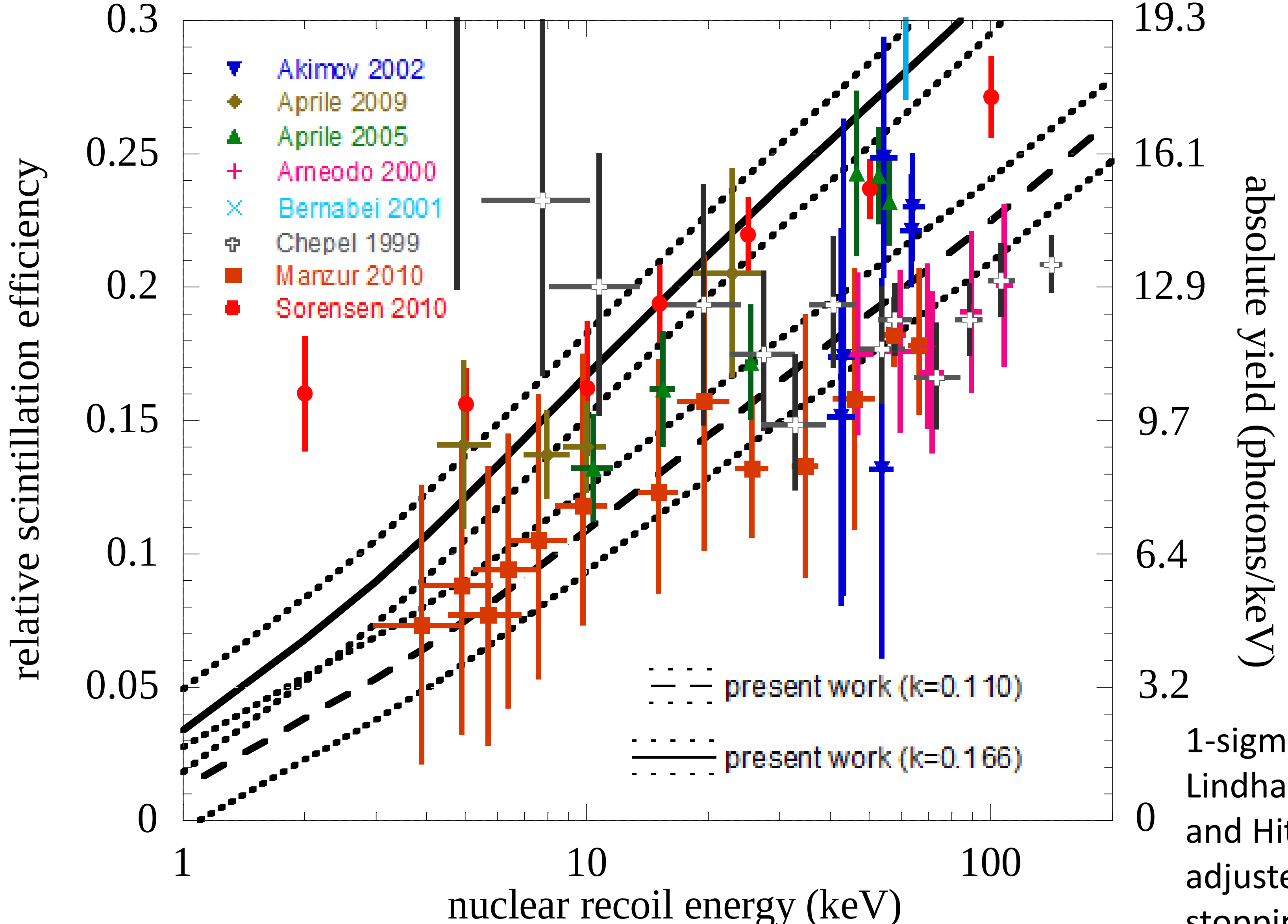
fake data (GEANT4 toy xenon model simulation) at the lower left. Spread dominated by stochastic individual dE/dx fluctuations





Asymmetrical shape reproduced with Monte Carlo! It is caused by characteristic x-rays indirectly produced by one parent gamma

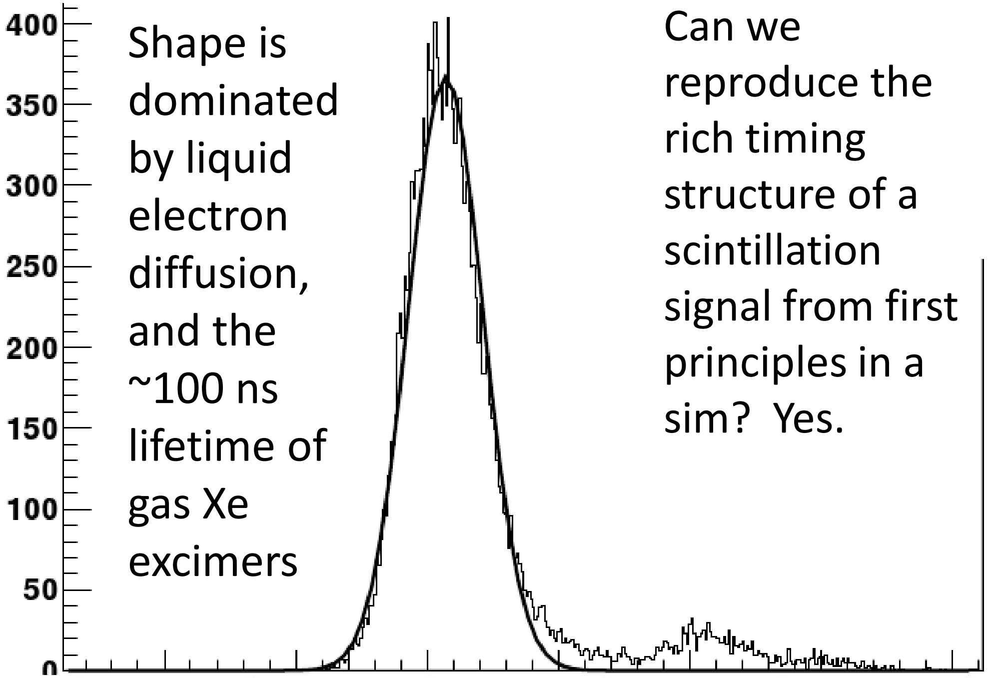
Switching Gears: Nuclear Recoil



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

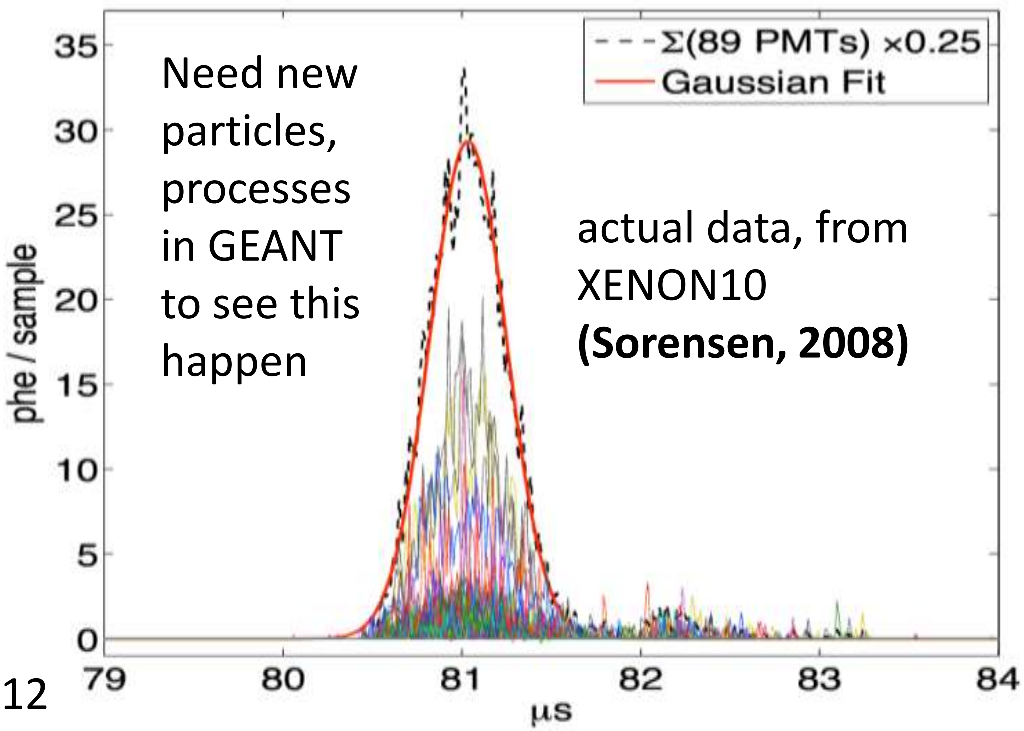
1-sigma bands for Lindhard (top) and Hitachi – adjusted (bottom) stopping powers

Understanding the Raw Pulse Shapes (S1, S2)



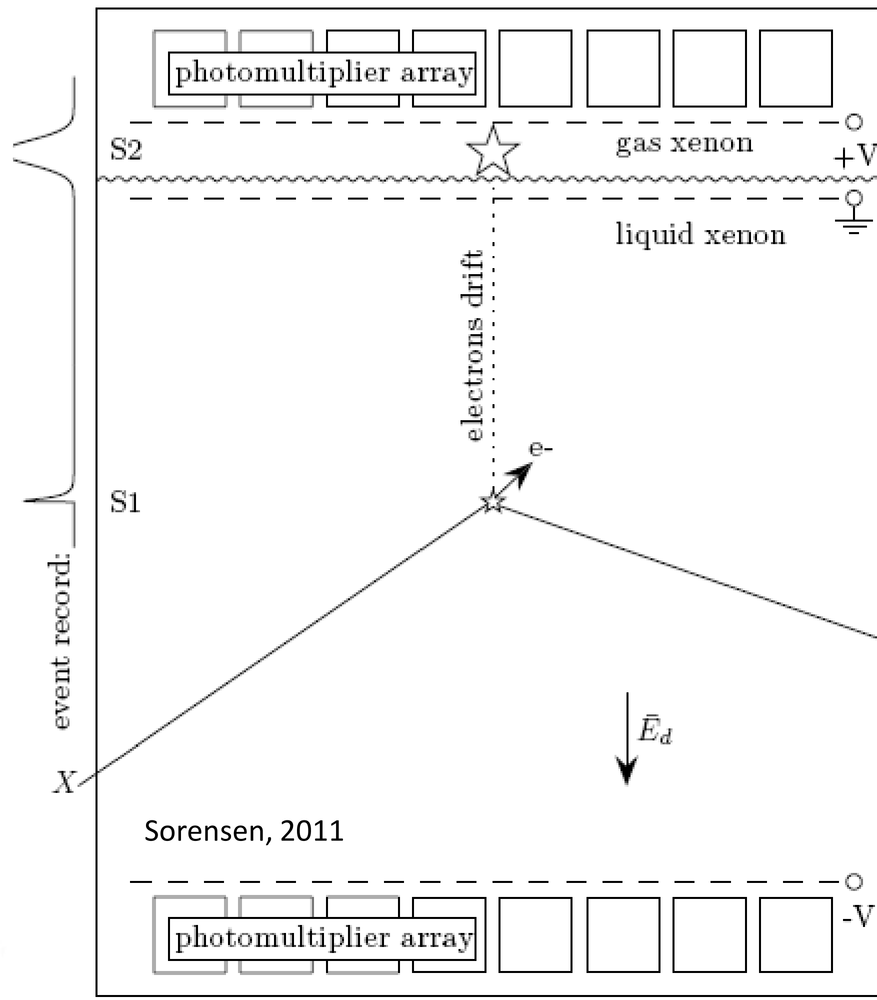
Shape is dominated by liquid electron diffusion, and the ~100 ns lifetime of gas Xe excimers

Can we reproduce the rich timing structure of a scintillation signal from first principles in a sim? Yes.



Need new particles, processes in GEANT to see this happen

actual data, from XENON10 **(Sorensen, 2008)**



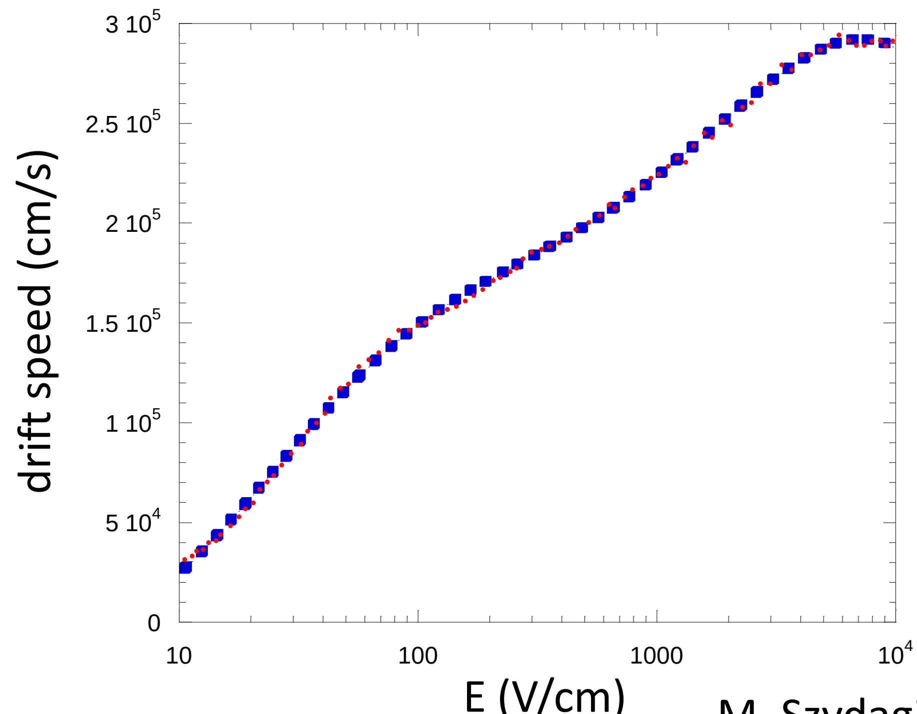
Sorensen, 2011

LXe Properties: The Finer Points

- We compiled all available (Xe) experimental data in the literature and performed a meta-analysis of it
- Scintillation wavelength is 174 nm (7.1 eV) with 11.5 nm FWHM, averaged over all results
- Compiled lifetimes, ratios for singlet, triplet states (unique for different interactions!)
- Studied the physics of electron drift so we can now simulate 2-phase detectors w/field well

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

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



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Status and Future

- Preparing upgrade for **G4Scintillation.cc** , speaking with GEANT about inclusion in next version
- Fully simulating DAQ chain (pulse shaping, etc.)
- Studying recombination fluctuations, Fano factor
- LUX will soon enjoy the first application of the work presented here for predicting new data
- 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 sim give reliable results
- Repeat: argon, neon – complete picture

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