



*A Symphony of
Scintillation*

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

Monte Carlo Code for Noble Scintillation and Ionization

Matthew Szydagis

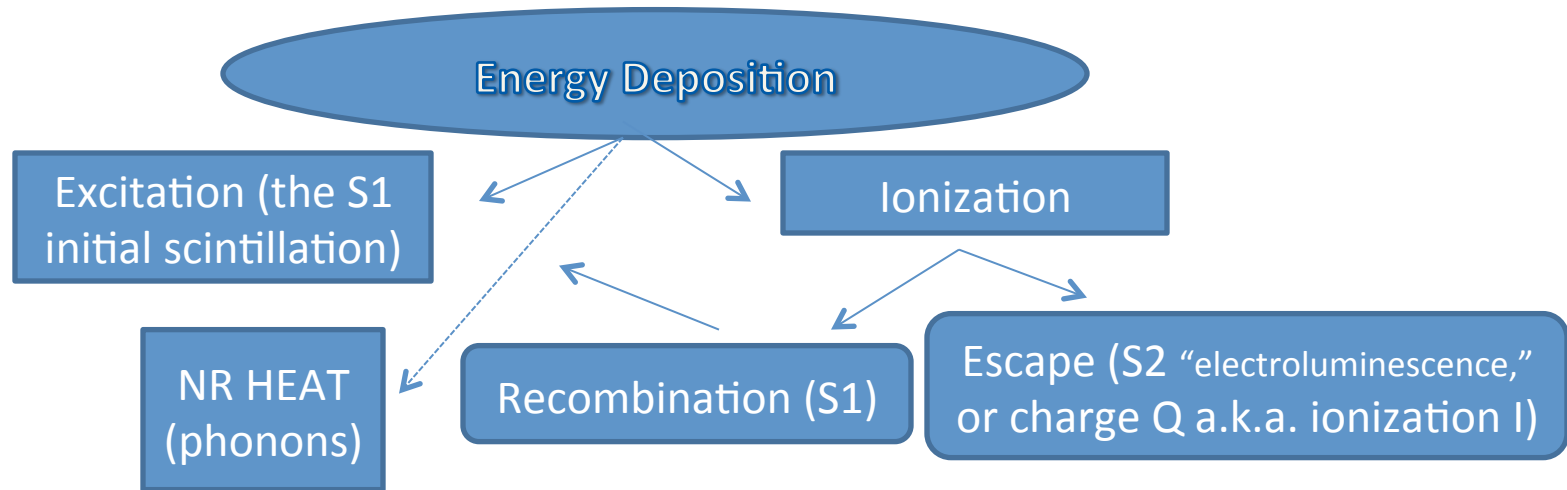
References

- There are now 3 NEST publications:
 - M. Szydagis et al., JINST 6 (2011) P10002. (**NEST: A Comprehensive Model for Scintillation Yield in Liquid Xenon**). 1st paper: 70+ references, some rare
 - M. Szydagis et al., JINST 8 (2013) C10003. (**Enhancement of NEST Capabilities for Simulating Low-Energy Recoils in Liquid Xenon**).
 - J. Mock et al., arXiv:1310.1117 (**Modeling Pulse Characteristics in Xenon with NEST**)...
- There is a comprehensive website which includes plots, and an archive of every NEST seminar, conference talk, or poster ever:
<http://nest.physics.ucdavis.edu/site/>

What is NEST?

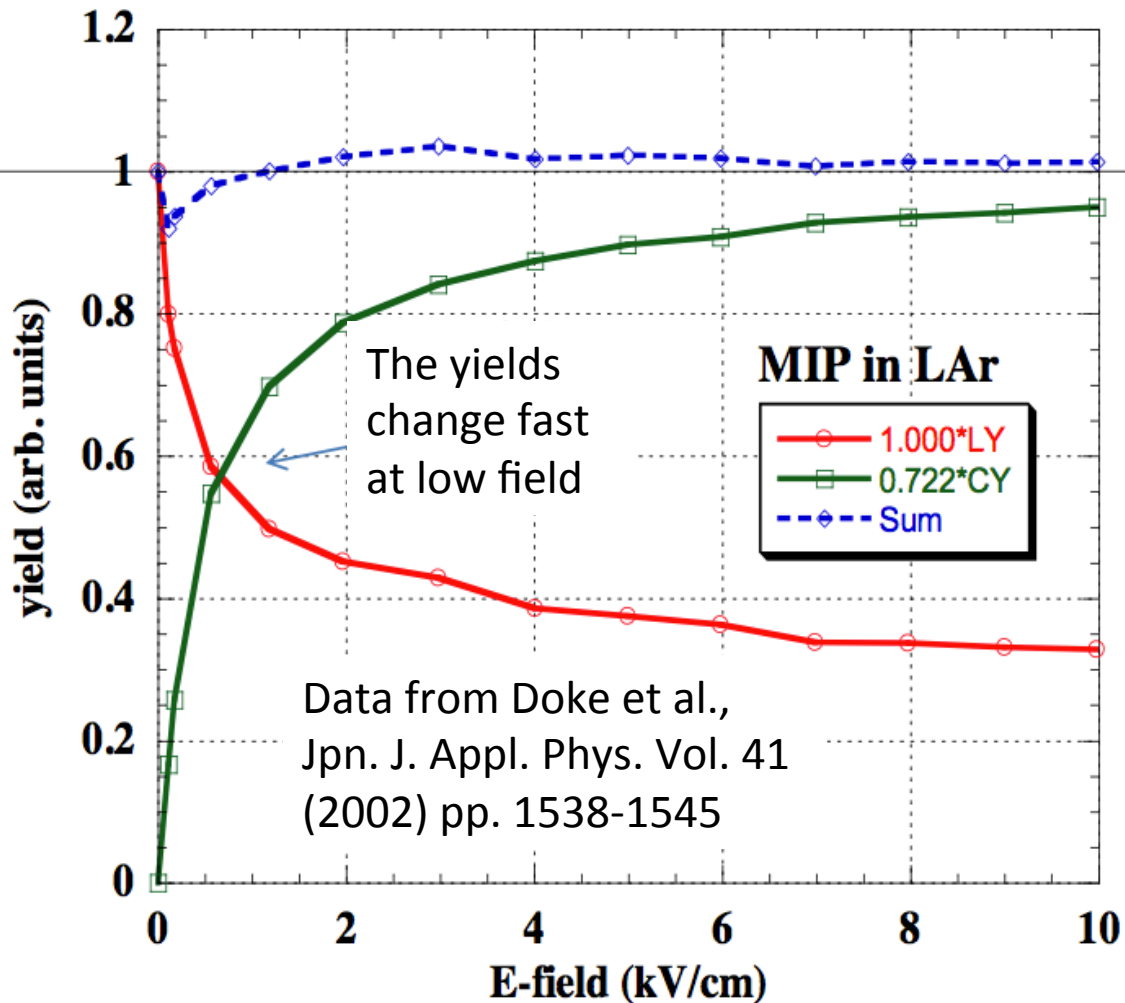
- The name refers to both a model (or, more accurately, a collection of models) explaining the scintillation and ionization yields of noble elements as a function of particle type (ER, NR, alphas), electric field, and dE/dx or energy
- ... as well as to the C++ code for Geant4 that implements said model(s), overriding defaults
- Has goal of providing a full-fledged MC sim with
 - Mean yields (light AND charge)
 - Energy resolution (includes BG discrimination)
 - Pulse shapes (S1 AND S2)
- Combed the wealth of data on noble elements and combined all of the physics learned

Basic Physics Principles



- Exciton-ion ratio 0.06 (173 K) for ER (~1 for NR)
- $S1 \neq$ energy: energy depositions divide into two channels, S1 and S2, non-linearly
- Nuclear recoils also have to deal with Lindhard*
* but it affects BOTH charge and light production

Anti-Correlation



- Proven in LXe before: “Correlated fluctuations between luminescence and ionization in liquid xenon,” Conti et al., Phys. Rev. B 68 054201 (2003).
- In LAr, anti-correlation between light and charge was not initially seen
- A re-analysis of old data shows this; DarkSide has seen it too (IDM '12)

Formulation of the Approach

- Cornerstone: one effective work function W for production of *either* a scintillation photon or an ionization electron. All others derive from it.

- $W_{LXe} = 13.7 \pm 0.2 \text{ eV}$

C.E. Dahl, Ph.D. Thesis, Princeton University, 2009

- Recombination different for short and long tracks

- Thomas-Imel “box” model TIB ($< O(10) \text{ keV}$)

- Doke’s modified Birks’ Law Doke et al., NIM A 269 (1988) p. 291

volume/bulk or
columnar
recombination \rightarrow

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

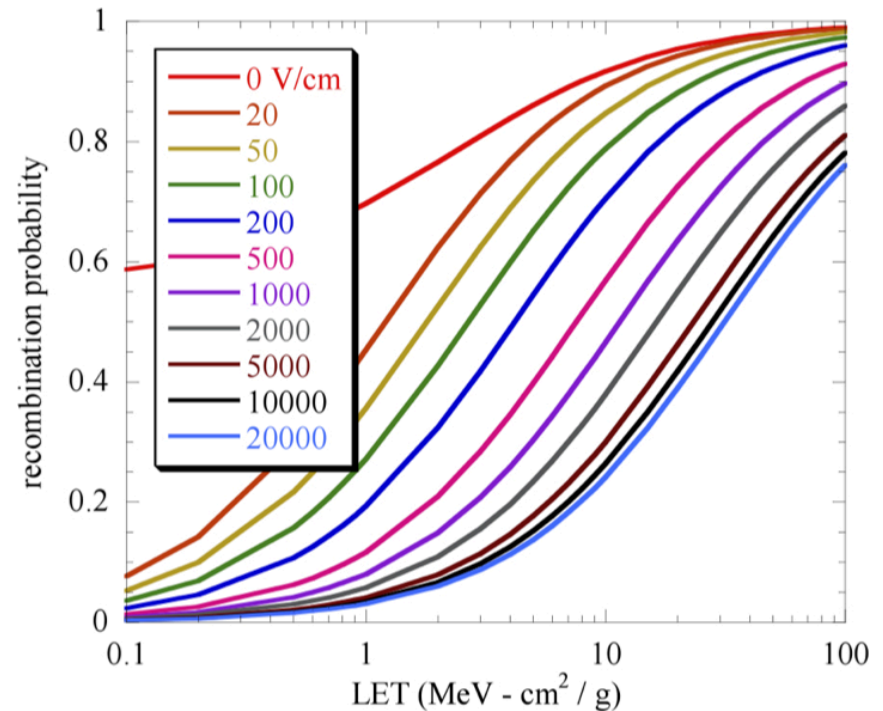
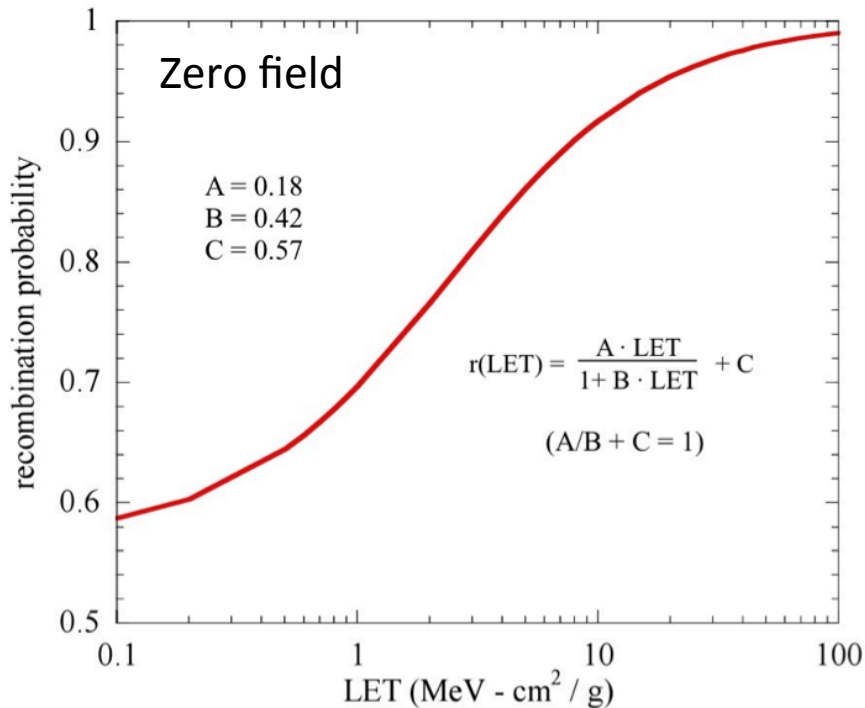
geminate (parent ion)

- Probability r makes for non-linear yield per keV

Energy Reconstruction

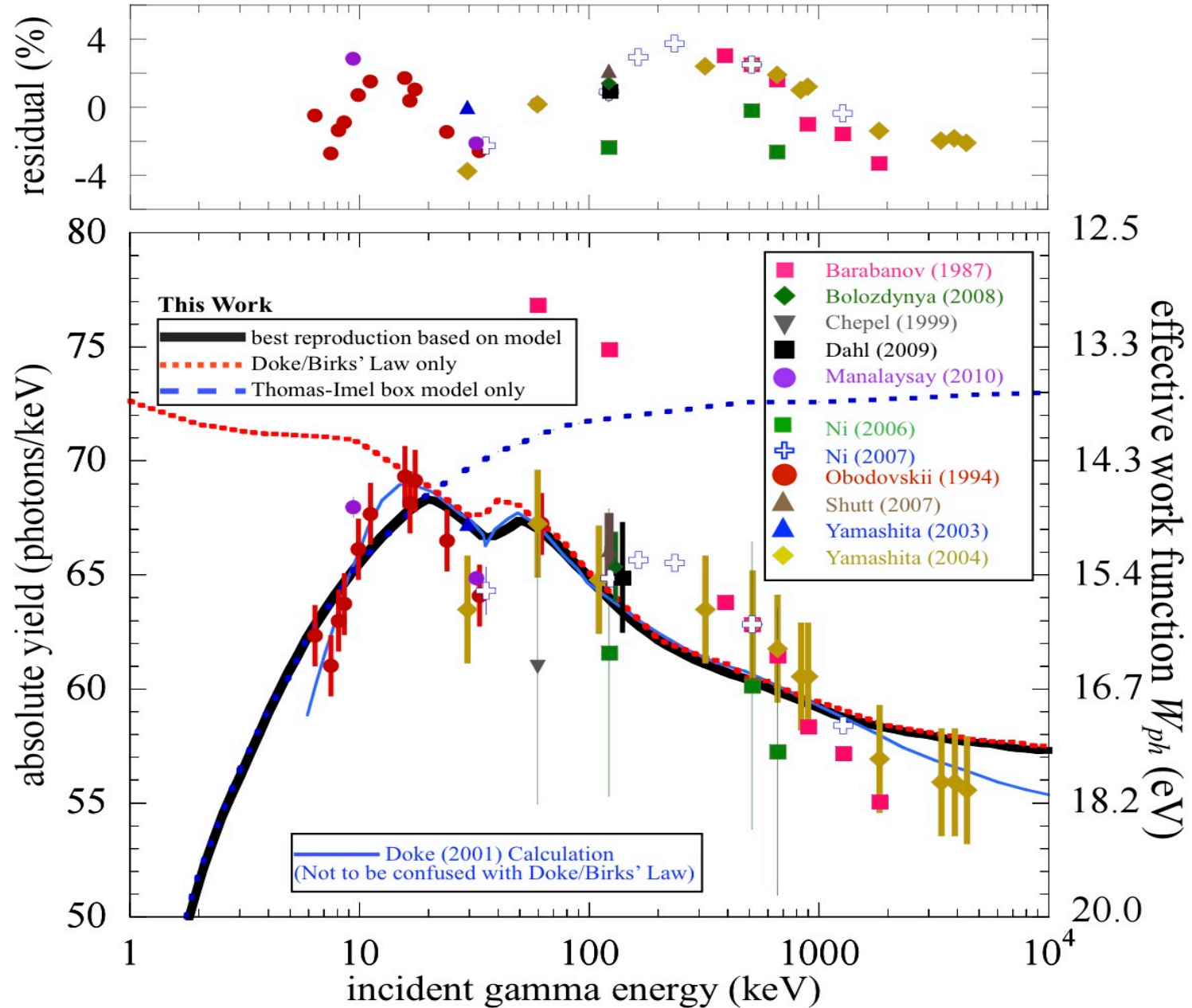
- $N_{\gamma} = N_{ex} + r N_i$ and $N_{e^-} = (1 - r) N_i$
- $E = (N_{e^-} + N_{\gamma}) W = (a S1 + b S2) W$
- 'a' and 'b' are simply the detection efficiencies for photons and electrons, respectively
- If floating, the values which optimize the resolution for a particular peak differ, and don't match efficiencies
 - Because the scintillation and ionization yields change with energy. Their ratio shifts.
 - Because S1 and S2 are affected differently by detector effects. (S1 has worse stats.)

Recombination Probability (LXe)



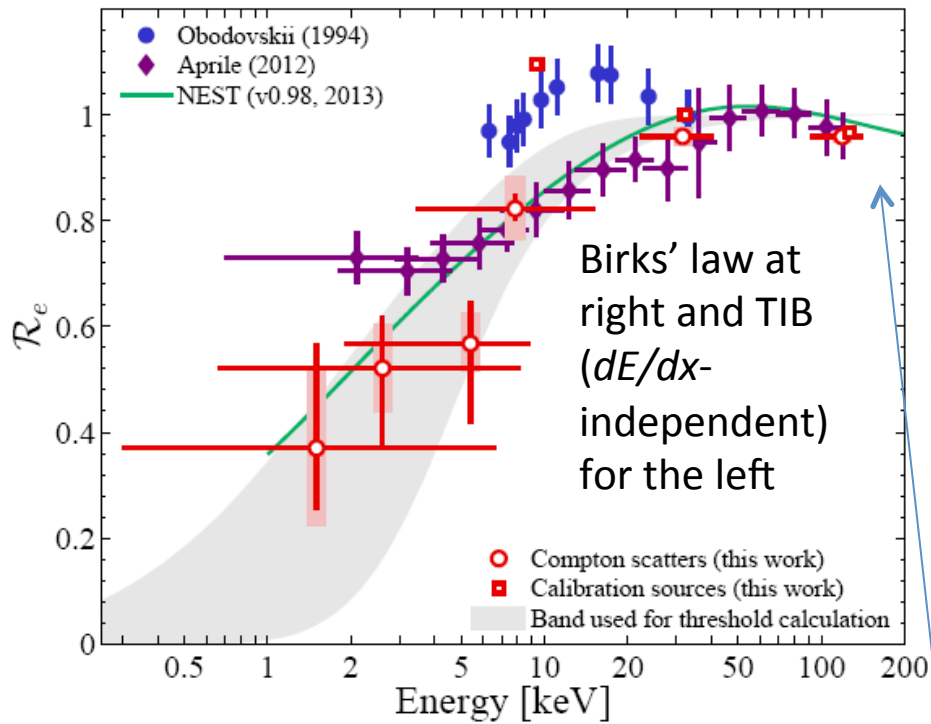
- An undifferentiated number of quanta is created, then fluctuated by the Fano Factor (0.03), for every energy deposition step in GEANT4
- Excitons and ions are separated binomially, and ions may recombine
- Function of dE/dx (Doke, above example) or N_i (TIB) with “constants” that vary with field, with Doke and TIB opposite in trend vs. energy

Absolute Zero-Field Light Yield vs. Energy

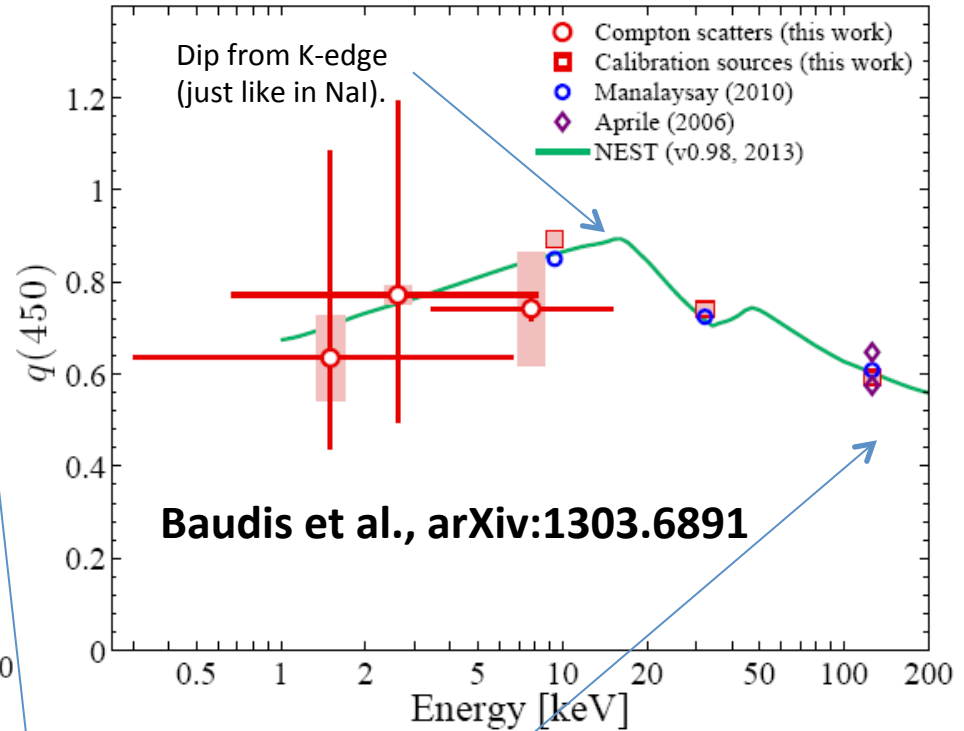


Relative Yield vs. Energy and Field

Zero field



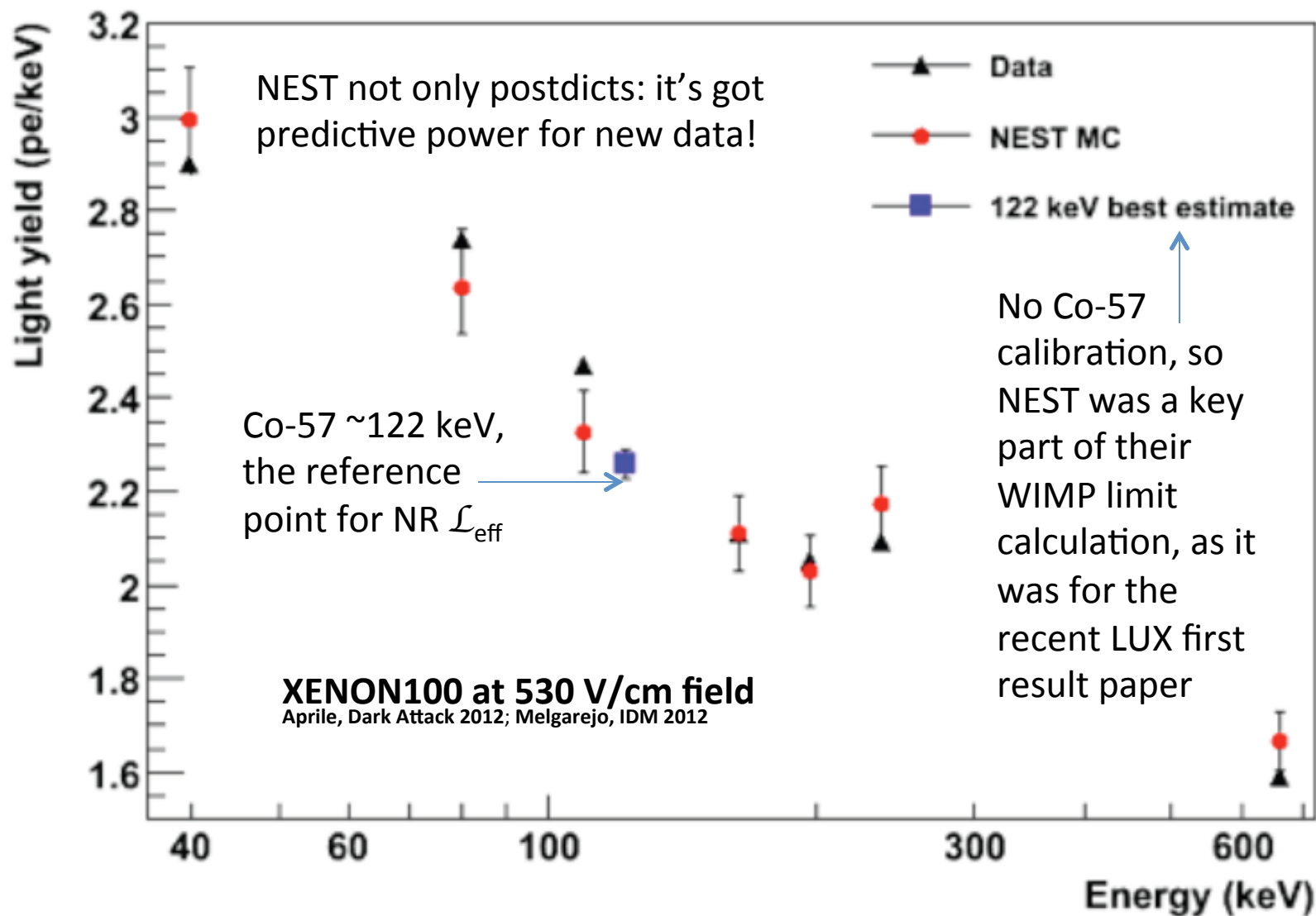
Non-zero field (450 V/cm)

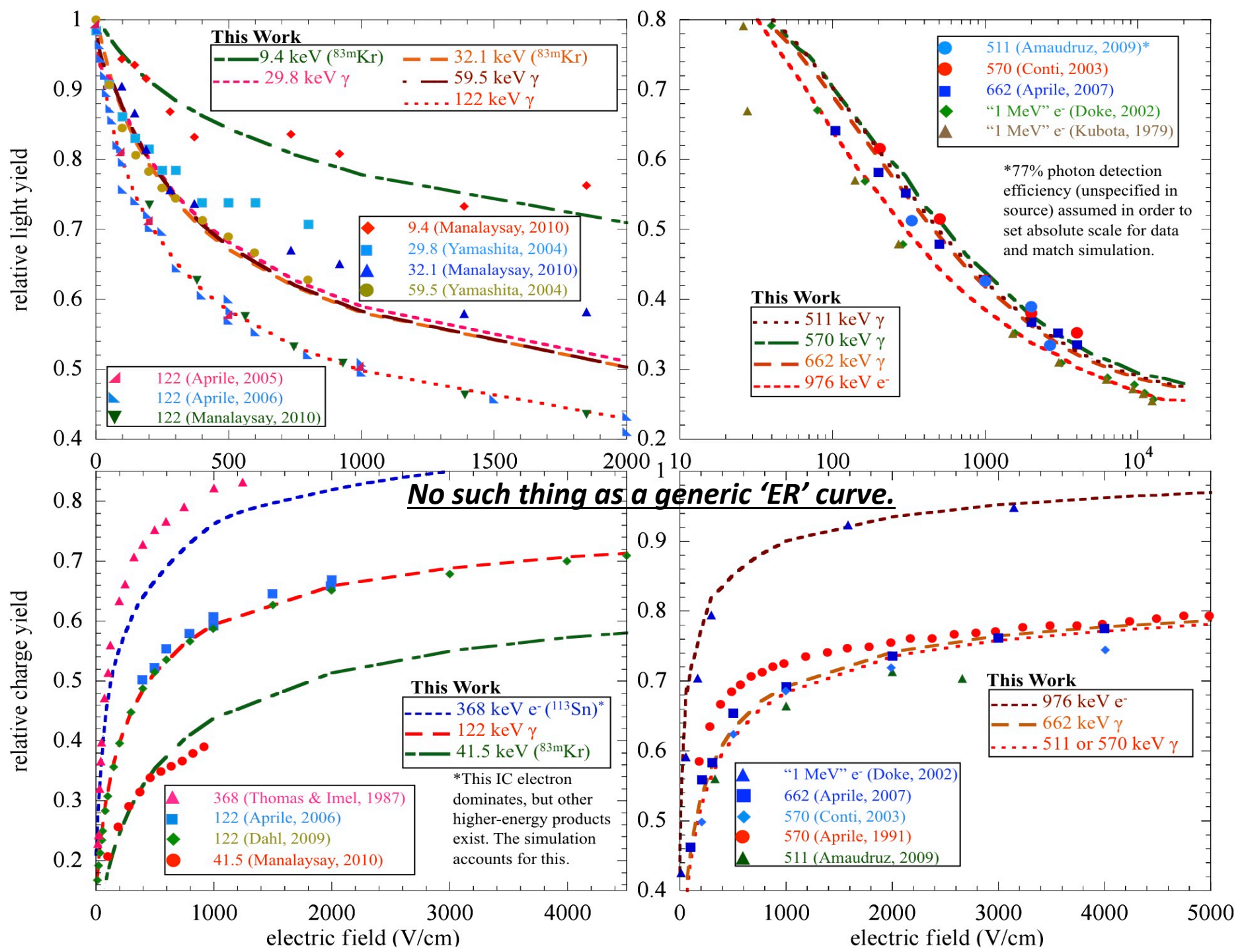


As the energy increases, dE/dx decreases, thus recombination decreases (less light ultimately, at the expense of more charge)

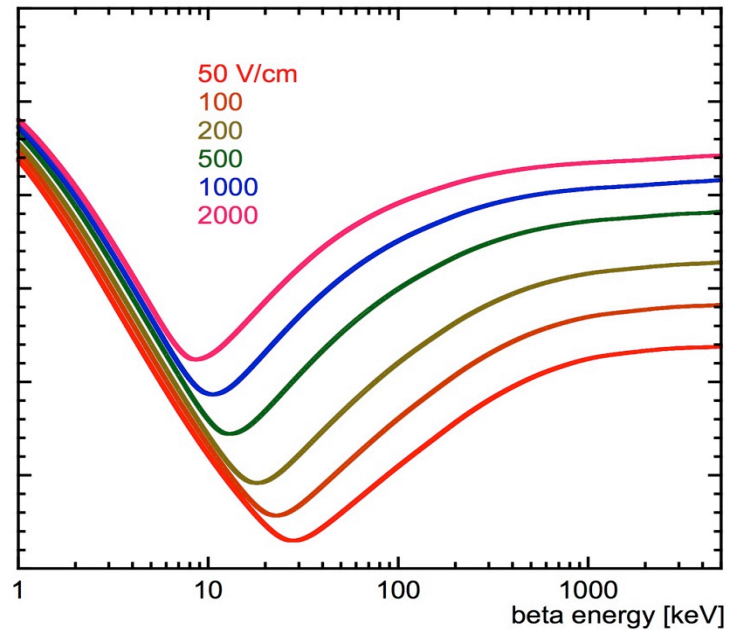
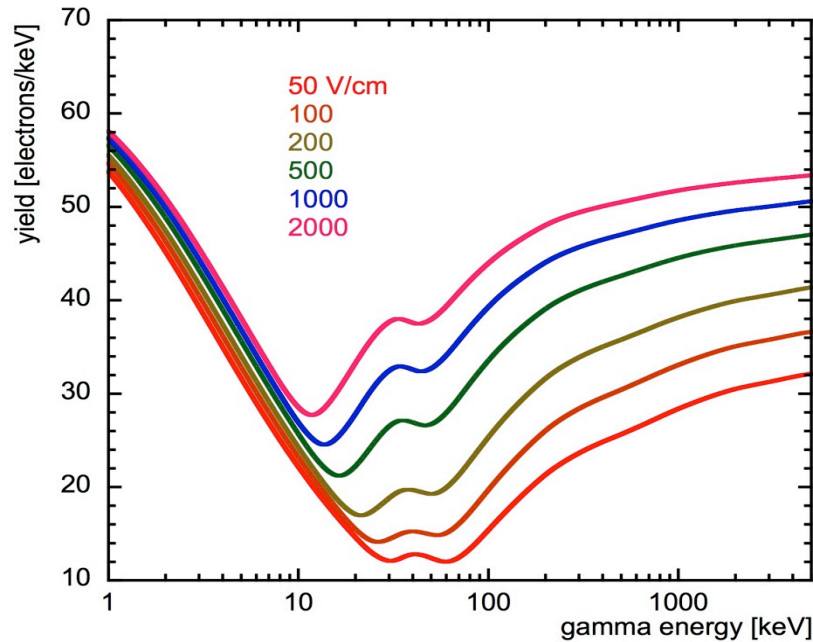
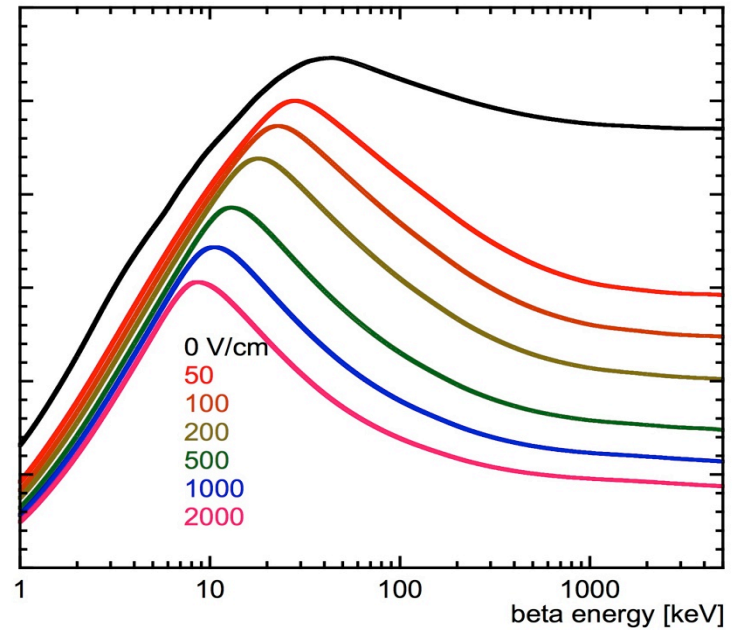
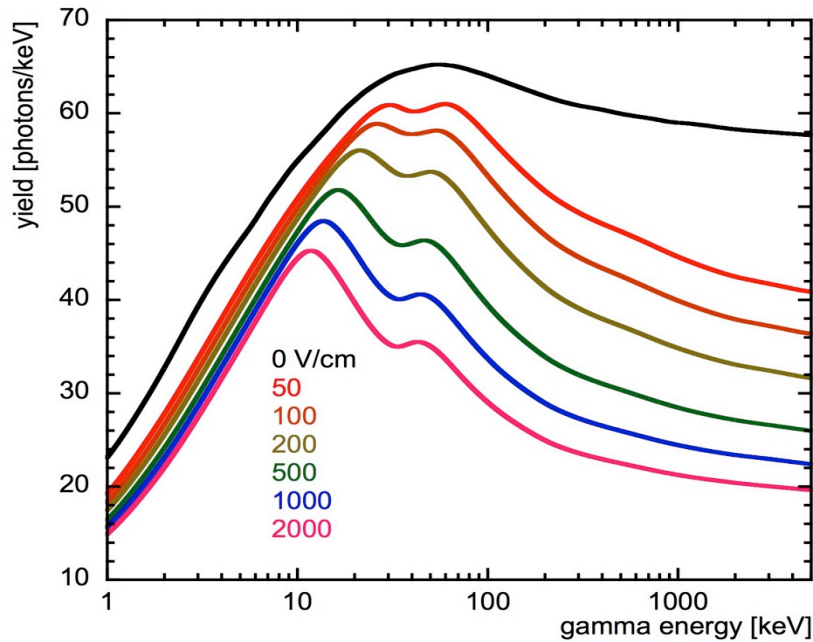
- NEST can translate yield assumptions between fields and energies

Relative Light Yield vs. Energy

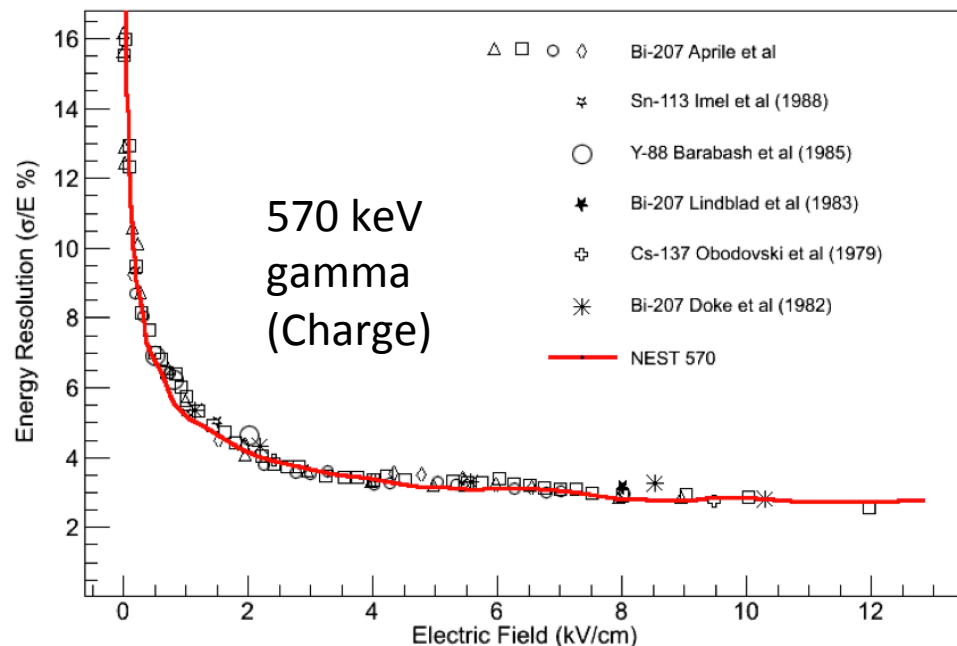
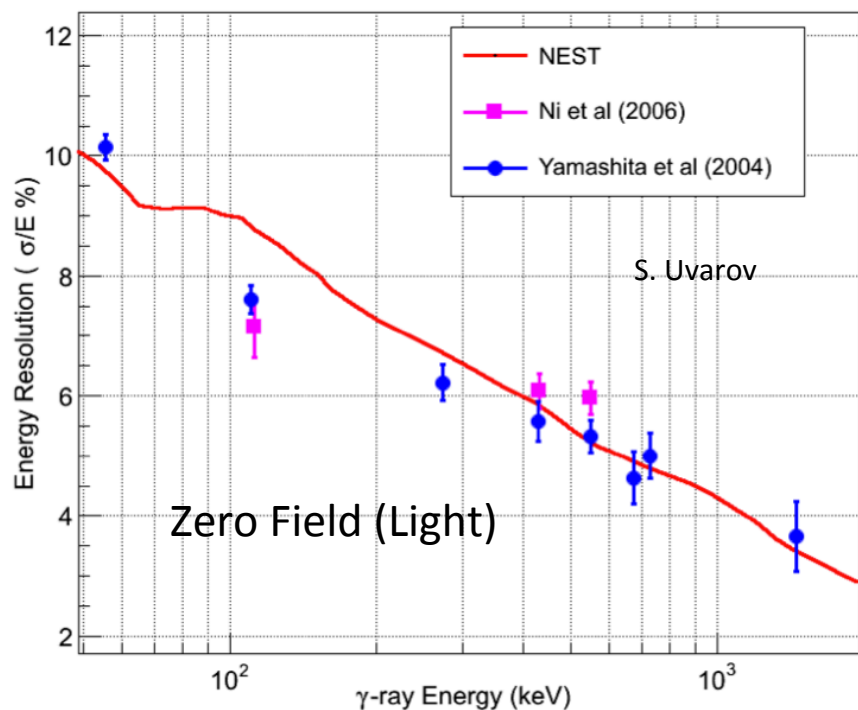




Absolute Yields vs. Field and Energy



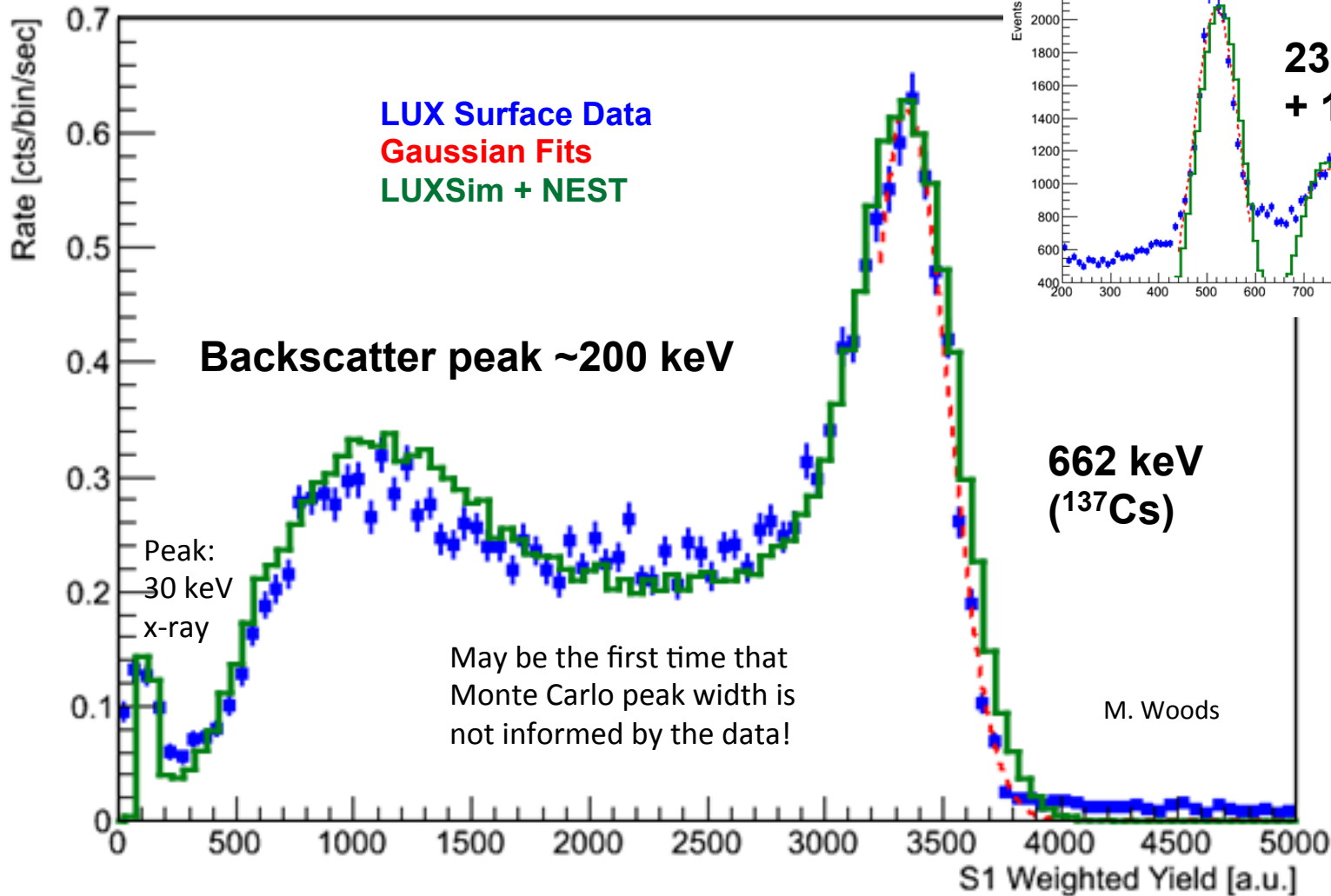
Energy Resolution: Light and Charge



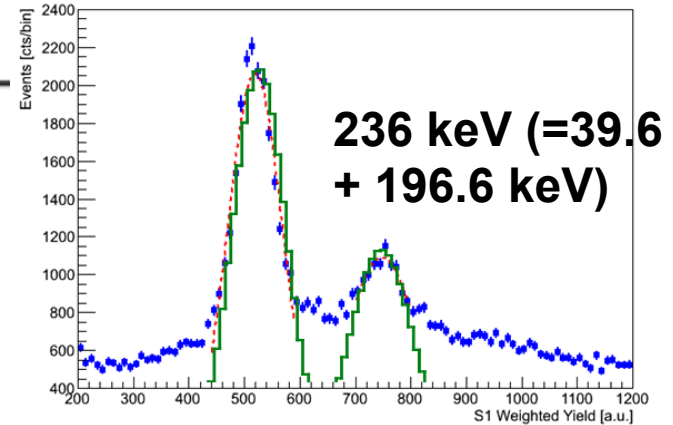
- Standard Fano factor left alone, but the recombination fluctuations modeled as worse than binomial, with a standard deviation of $\sqrt{F_e N_{e^-}}$
- An ansatz solution (seeking justification) that is energy-independent (almost), but electric field-dependent -- not fixed at 20 as in Conti et al.
- Effect applied per interaction site, and disappears as the field goes to infinity, but starts high ($F_e > 400$ @ZF) and disappears at low energies

Energy Resolution: Light

Source: the LUX engineering run paper

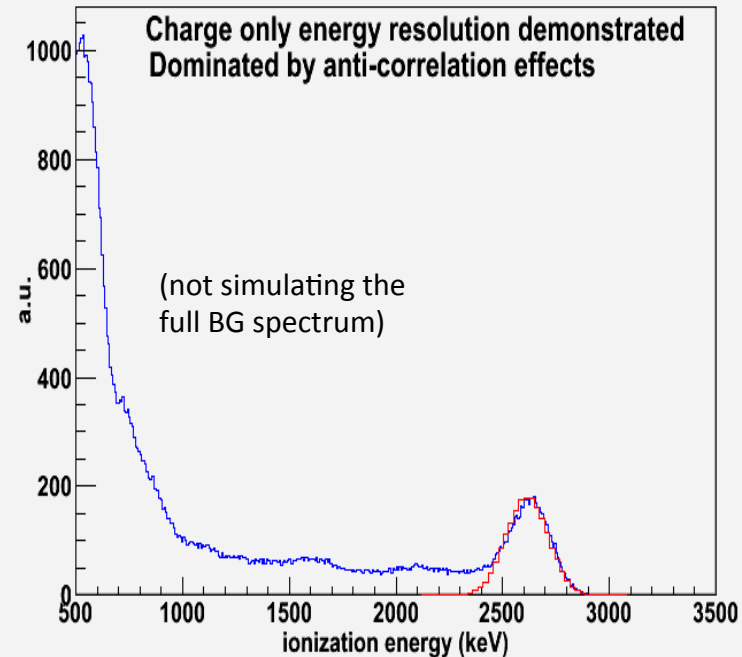
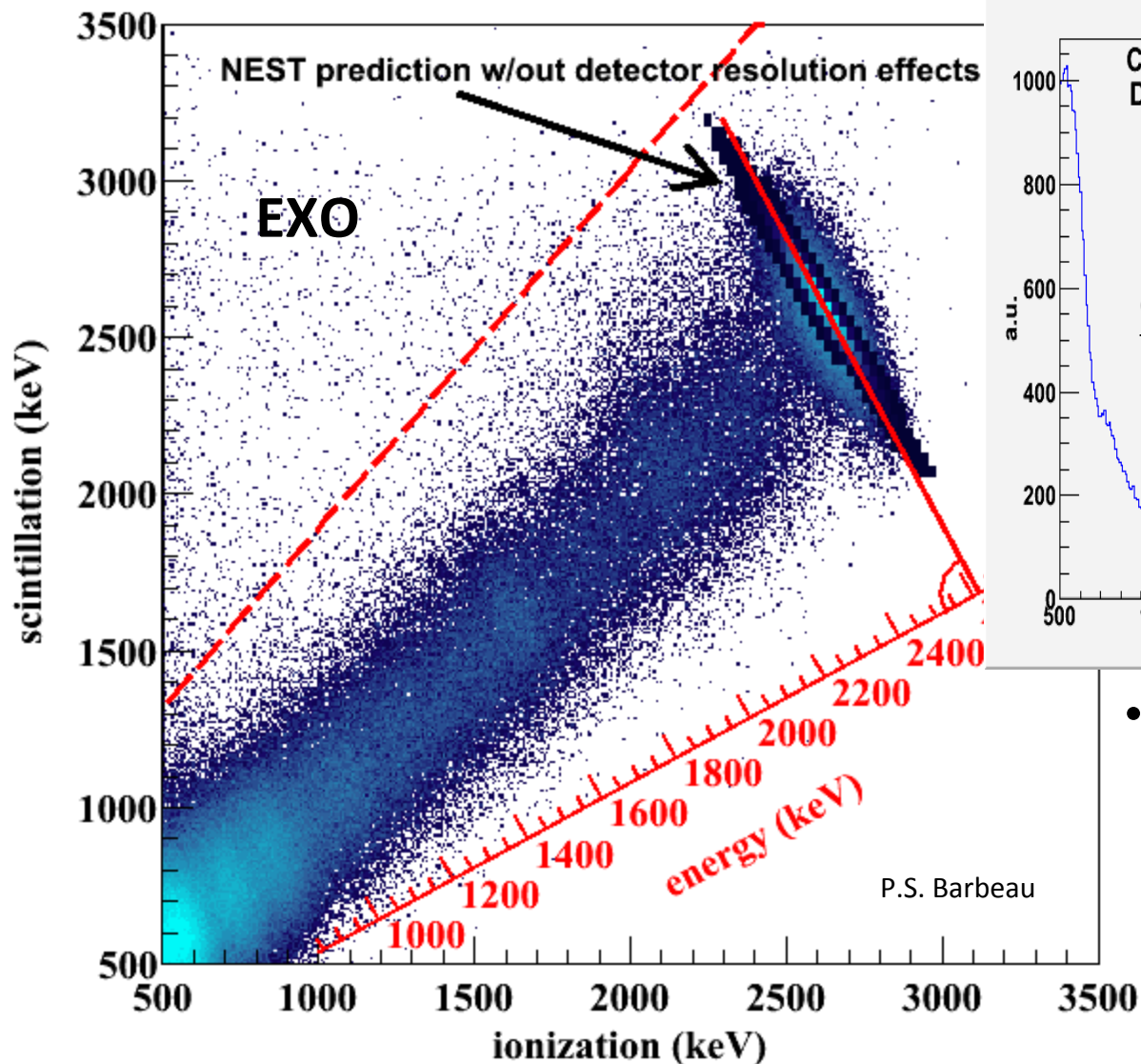


164 keV



Fit at same time with same model

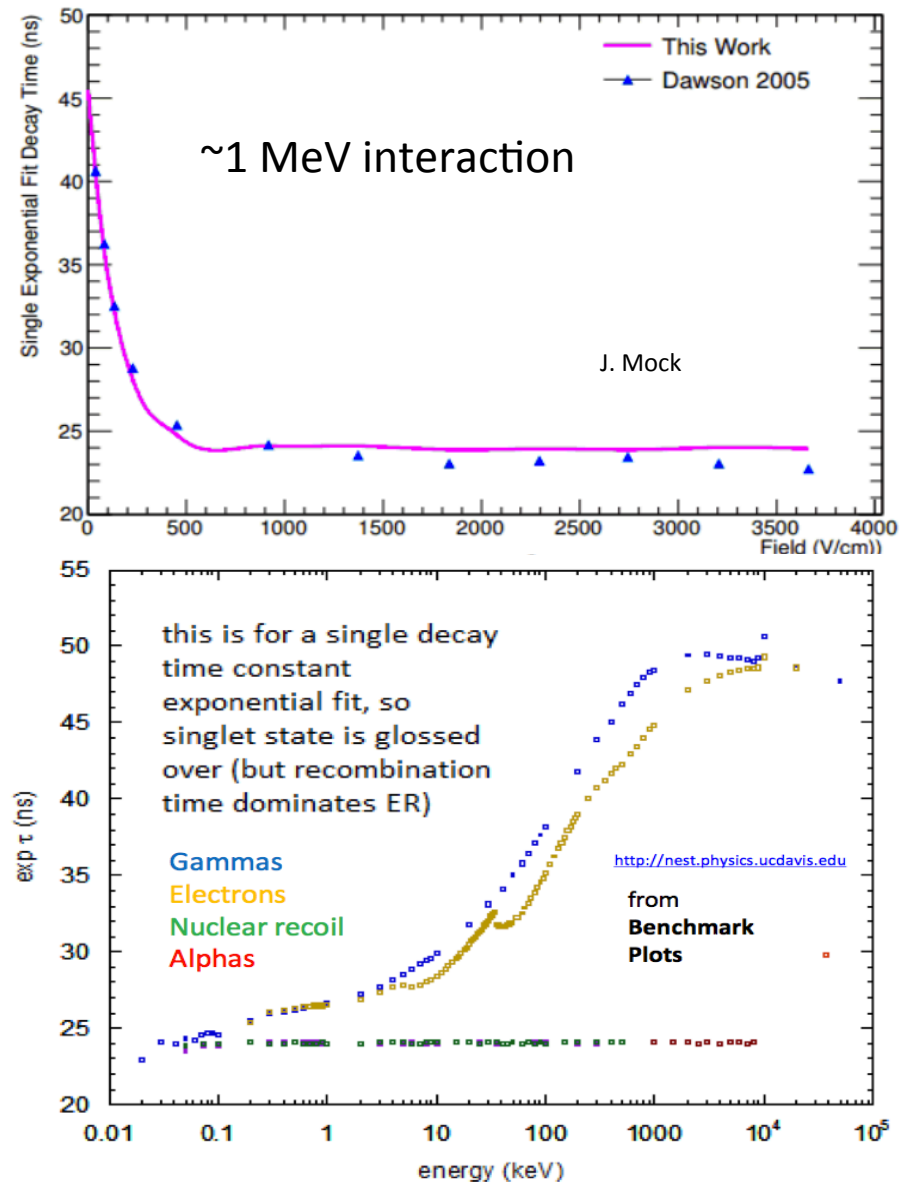
Combined Energy Resolution



- Prediction for a field never before studied (376 V/cm) and a new energy (2.6 MeV gammas, whereas vetted at 570 keV)

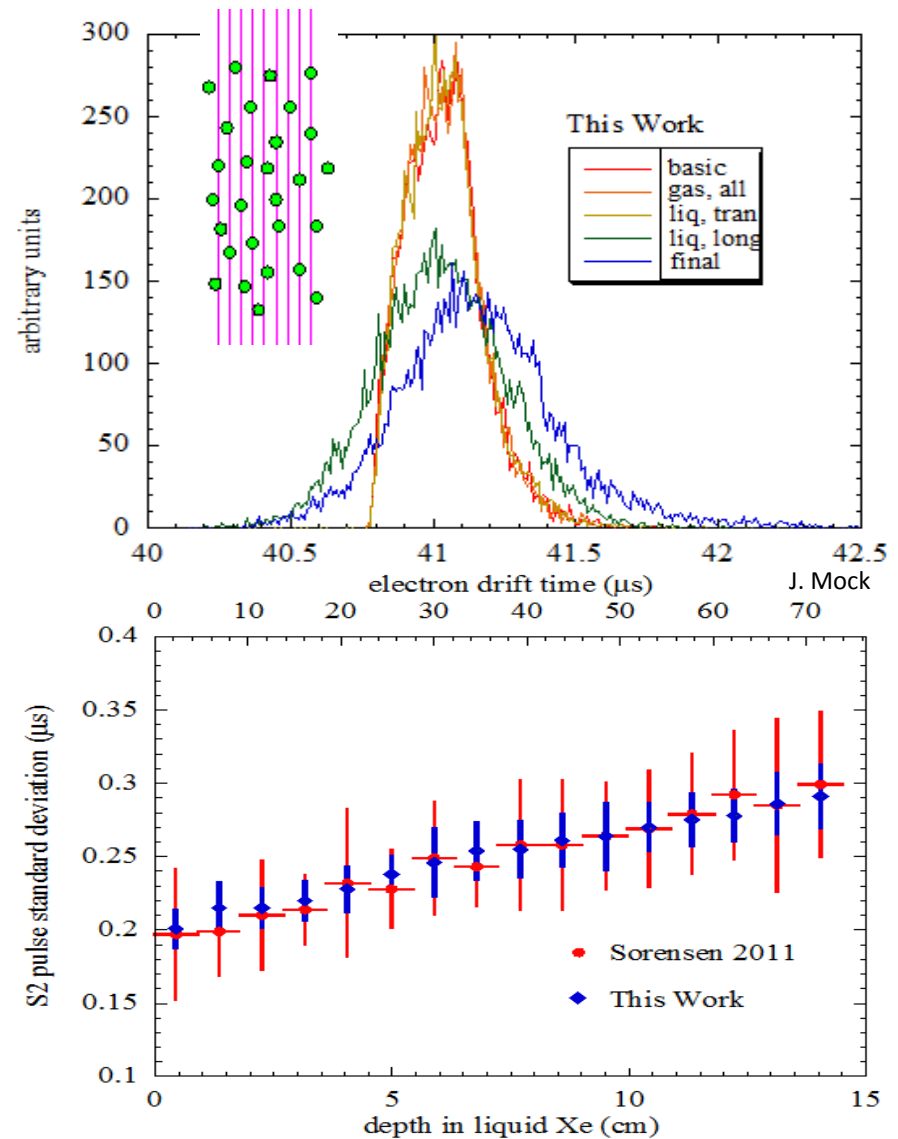
Pulse Shape (S1)

- The differences between ER and NR disappear with higher fields
- Also disappear at lower energies (bad for PSD)
- Two exponential time constants corresponding to the triplet and singlet Xe dimer states, but the triplet time dominates
- Ratio of populated states a function of particle type
- Recombination goes as $1 / \text{time}$, but time constant not fixed (related to the LET and electric field)



Pulse Shape (S2)

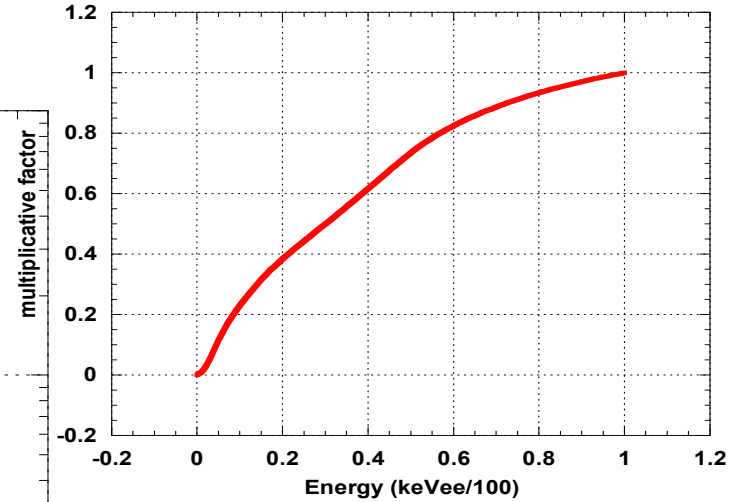
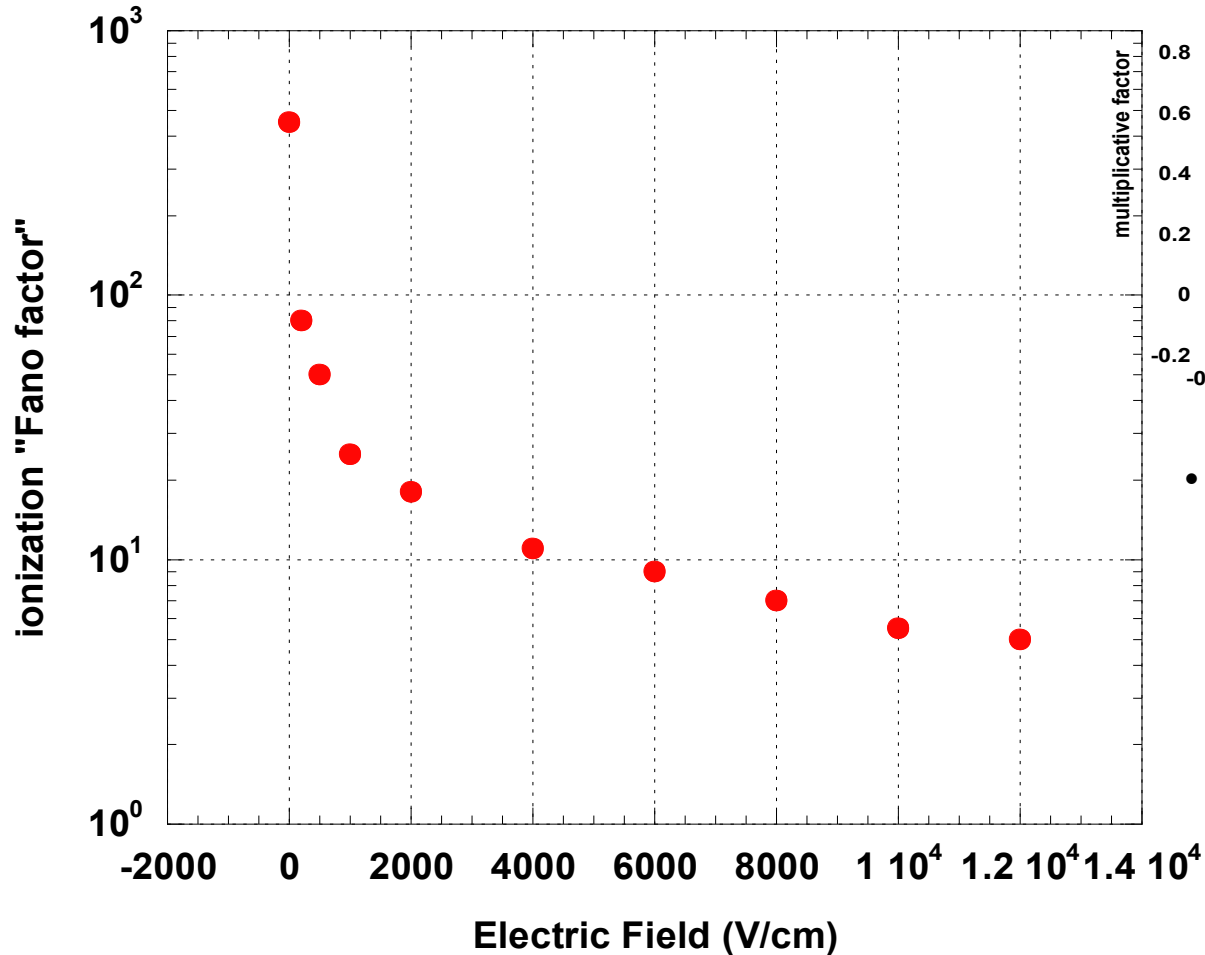
- New particle type for drift electrons
- *Can* do 3-D field mapping
- Long list of effects included
 - Drift speed (liquid, gas)
 - Different triplet (~100 ns!) and singlet decay times in the gas phase
 - Diffusion constants (transverse and especially longitudinal)
 - Electron trapping time at gas / liquid interface prior to extraction
- Can now reproduce S2 width versus depth without any empirical-only factor



Conclusions

- Model and software NEST has a firm grasp of microphysics.
- **Though NEST doesn't track individual atoms or excimers, it's not far from a fully first principles approach, as it considers the excitation, ionization, recombination process, resorting to interpolative splines as indirect fits or not at all**
- Extensive empirical verification with past data undertaken using multiple results instead of only one experiment
- **NEST is intricate, and it is not trivial to convey all of the subtleties, but the noble life is an intricate one. Lots of things historically thought of as constant found to depend on field, energy, density, etc. such as scintillation yield**
- Currently, all parameters are physically well-motivated except for the (large) size of the recombination fluctuations in LXe

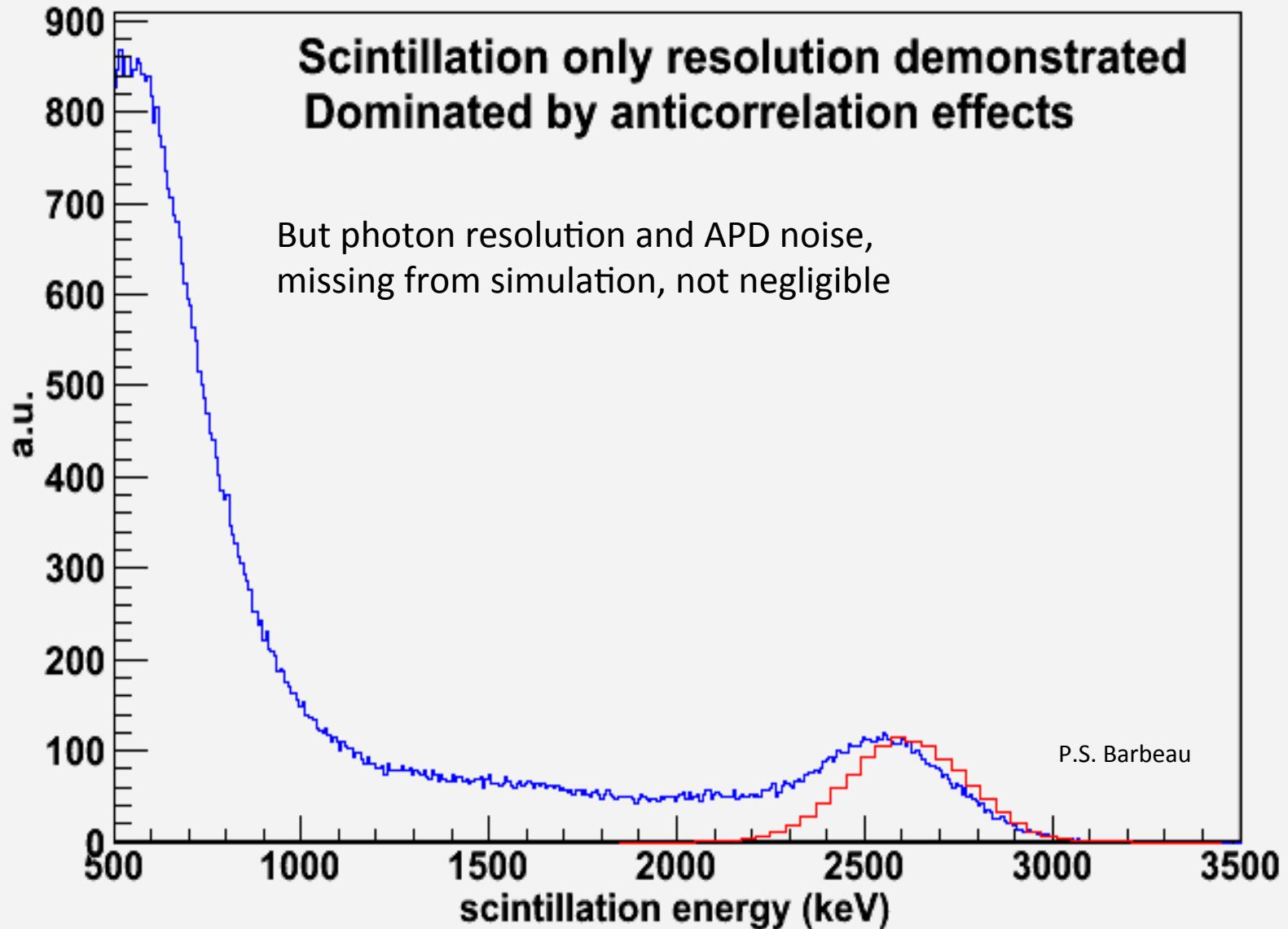
Recombination Fluctuation



- The anomalously high recombination fluctuations at high energies, where F_e is $O(10-100)$, are smoothly extrapolated down to 0 additional fluctuation (i.e., binomial only) at 0 energy (using 876 V/cm Dahl data to ground the NEST model)

Scintillation only resolution demonstrated Dominated by anticorrelation effects

But photon resolution and APD noise,
missing from simulation, not negligible



P.S. Barbeau