A Symphony of Scintillation

Noble **E**lement **S**imulation **T**echnique, A Model of Scintillation and Electroluminescence in Noble Elements

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

LLNL Advanced Detectors Group (ADG) Monthly Meeting, Livermore, CA, Thursday 12/13/2012

The People of the NEST Team

UC Davis and LLNL

A small but passionate group of individuals who love their work

<u>Postdocs</u>

Matthew Szydagis*

<u>Faculty</u>

Mani Tripathi

<u>Physicists</u>

Kareem Kazkaz

<u>Graduate Students</u>

Jeremy Mock

Nick Walsh

Mike Woods

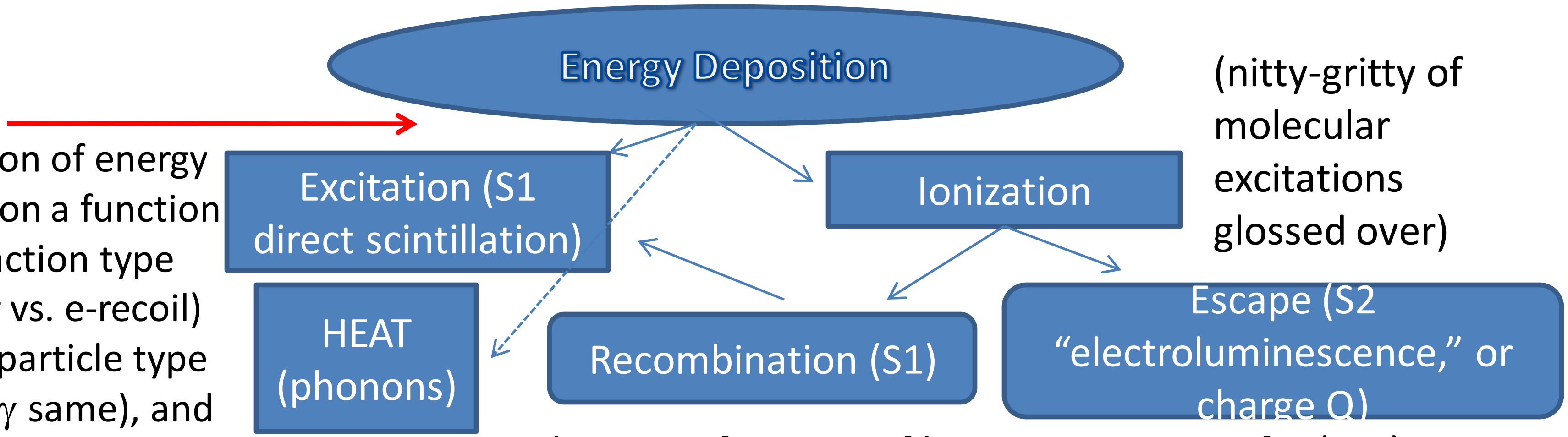
Why simulate scintillating noble elements well?

- 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 ($0\nu\beta\beta$, $2\nu\beta\beta$) projects, too
  - NEXT, EXO (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 full-fledged simulation based on a 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 a comparable page for simulations
- Bring added realism to the simple model that is present now in Geant4 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 the sake of LUX)

Basic Physics Principles



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

(nitty-gritty of molecular excitations glossed over)

(the infamous $\mathscr{L}_{eff}$ 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

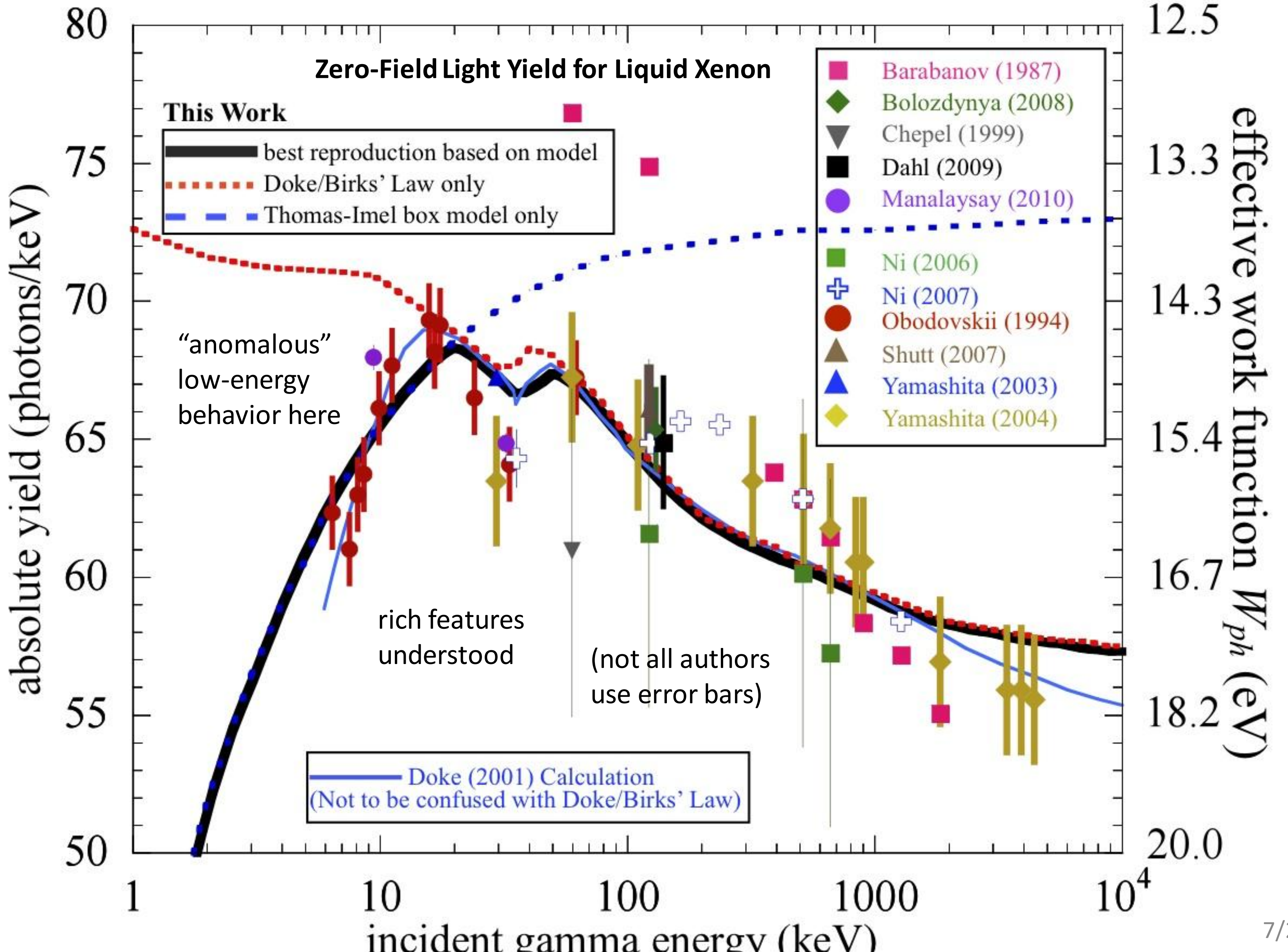
- Heat loss for nuclear recoils (Lindhard effect), while electron recoils relatively easier to deal with
- Start simple: no exotic energy loss mechanisms (like “bi-excitonic” collisions). Explains the data?

Basic Physics Principles

- Cornerstone: There is 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
  – Thomas-Imel "box" model (below *O*(10) keV)
  – Doke Modified Birks' Law
- Recombination probability makes for non-linear yield: 2x energy does not mean 2x light + charge
- Excellent vetting against much past data

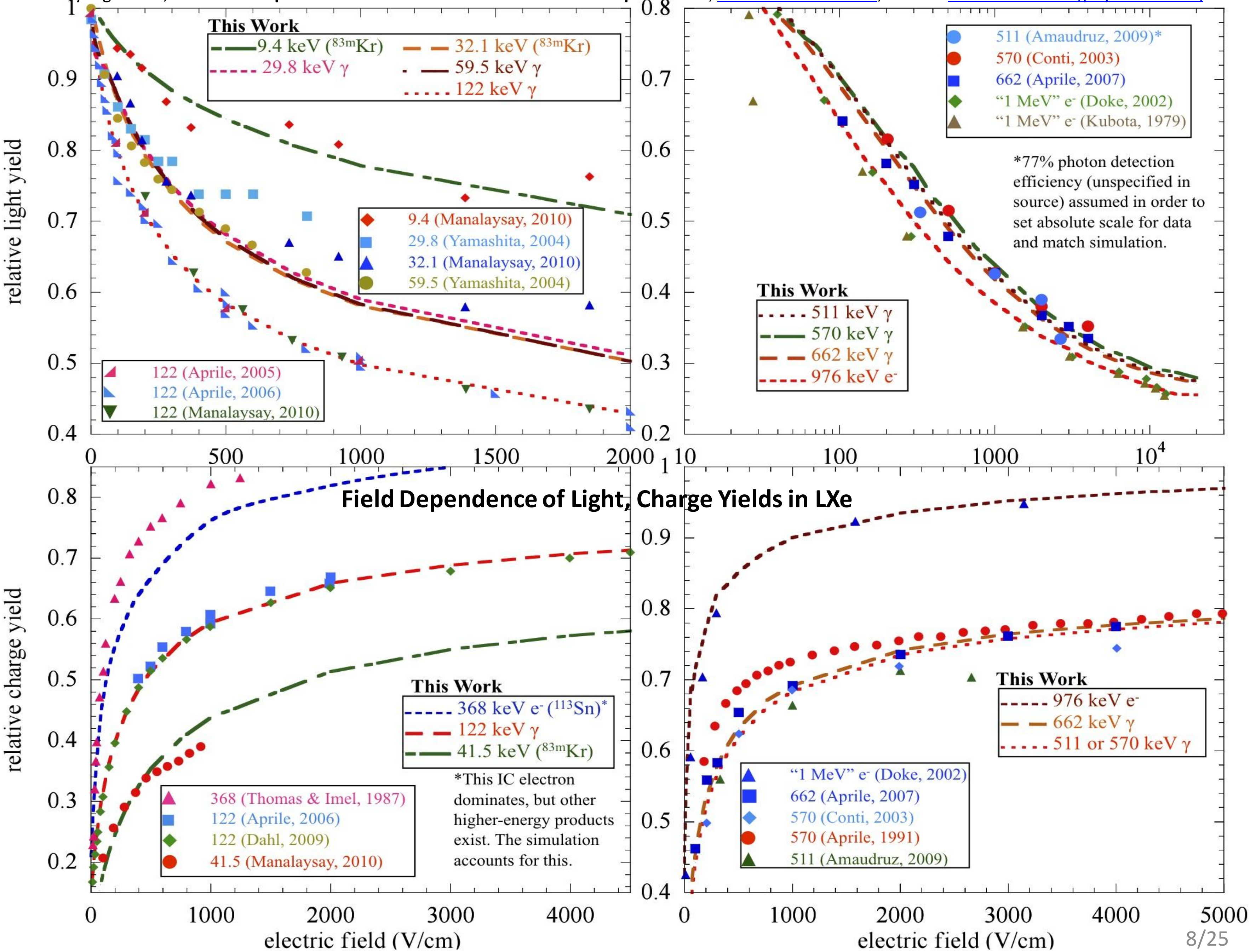
Putting it All Together to Predict Yield

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]]()



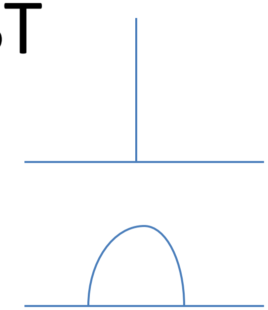
Szydagis et al., **NEST: A Comprehensive Model for Scintillation Yield in Liquid Xenon**, 2011 JINST 6 P10002; e-Print: arxiv:1106.1613 [physics.ins-det]

Field Dependence of Light, Charge Yields in LXe

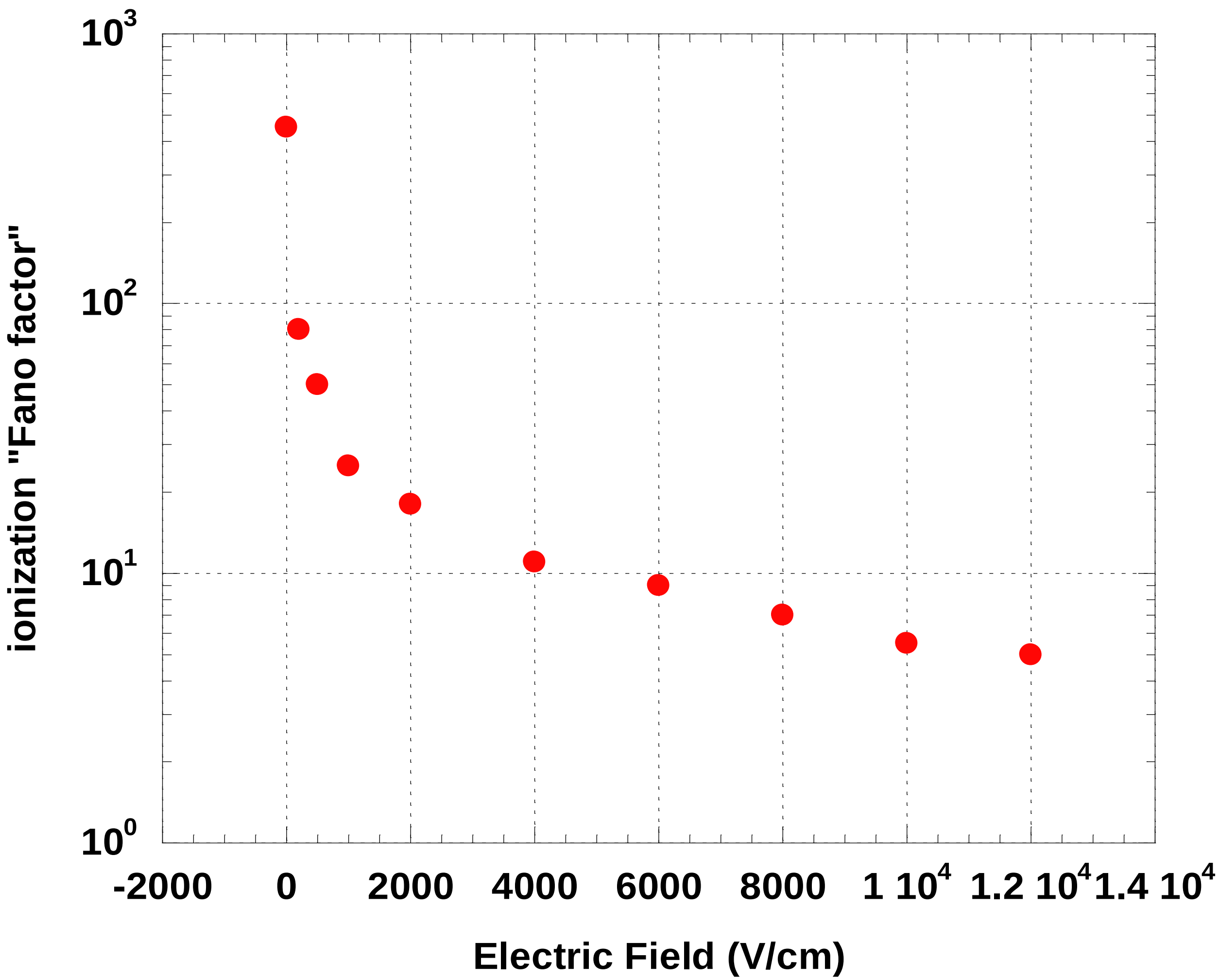


Energy Resolution

- Long list of effects now included in NEST
  - Fano factor (very small effect)
  - N_{ex} vs. N_i (binomial fluctuation)
  - Recombination fluctuations
    - Binomial (to recombine, or not to recombine)
    - “Extra,” special (next slide)
  - Geant4 stochastic dE/dx variation
  - Particle track history (also Geant4)
  - Finite quantum efficiency
  - Imperfect light collection (Geant4)
- Angle of particle track with respect to electric field vector not yet included

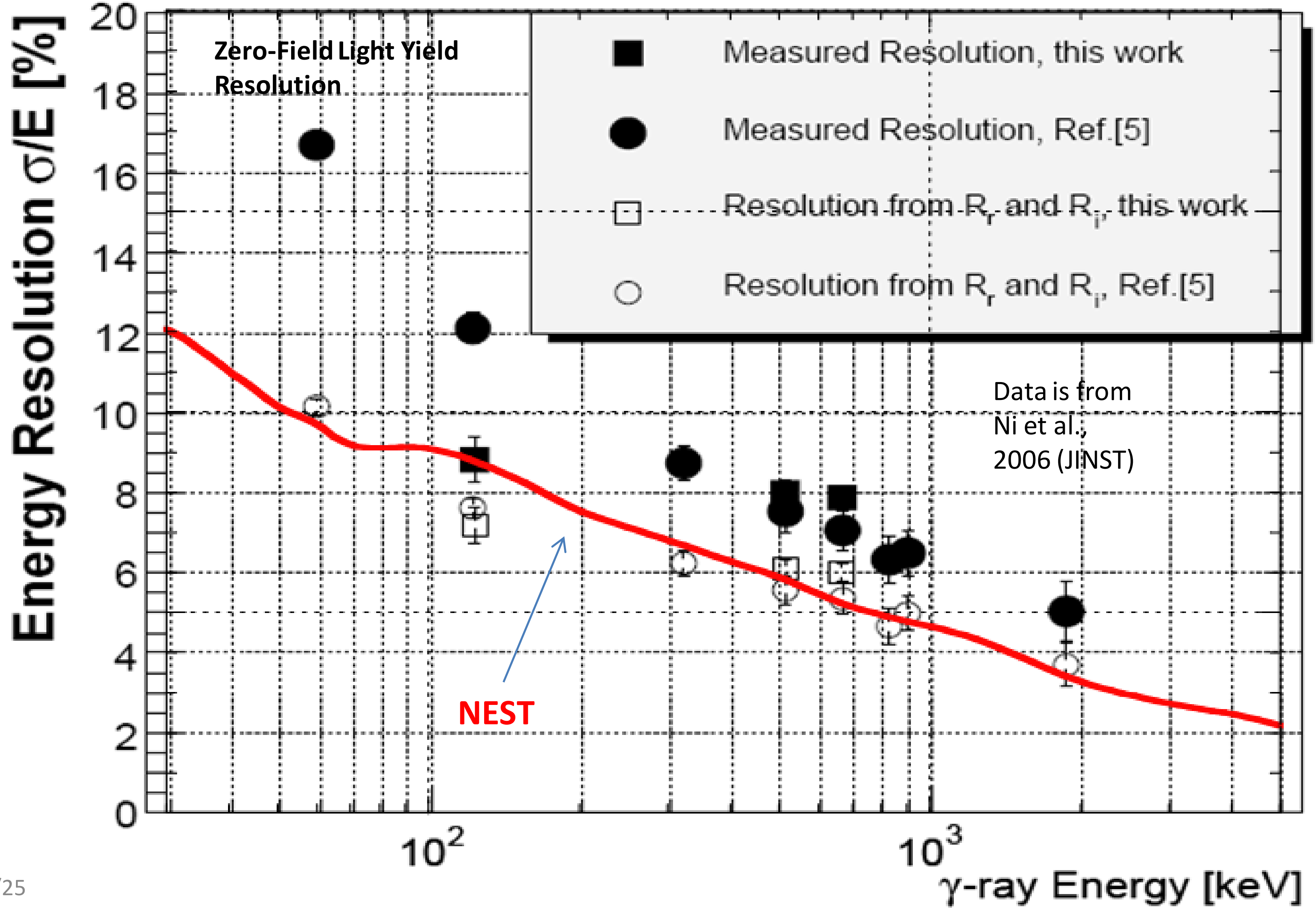


Recombination Fluctuations: Model

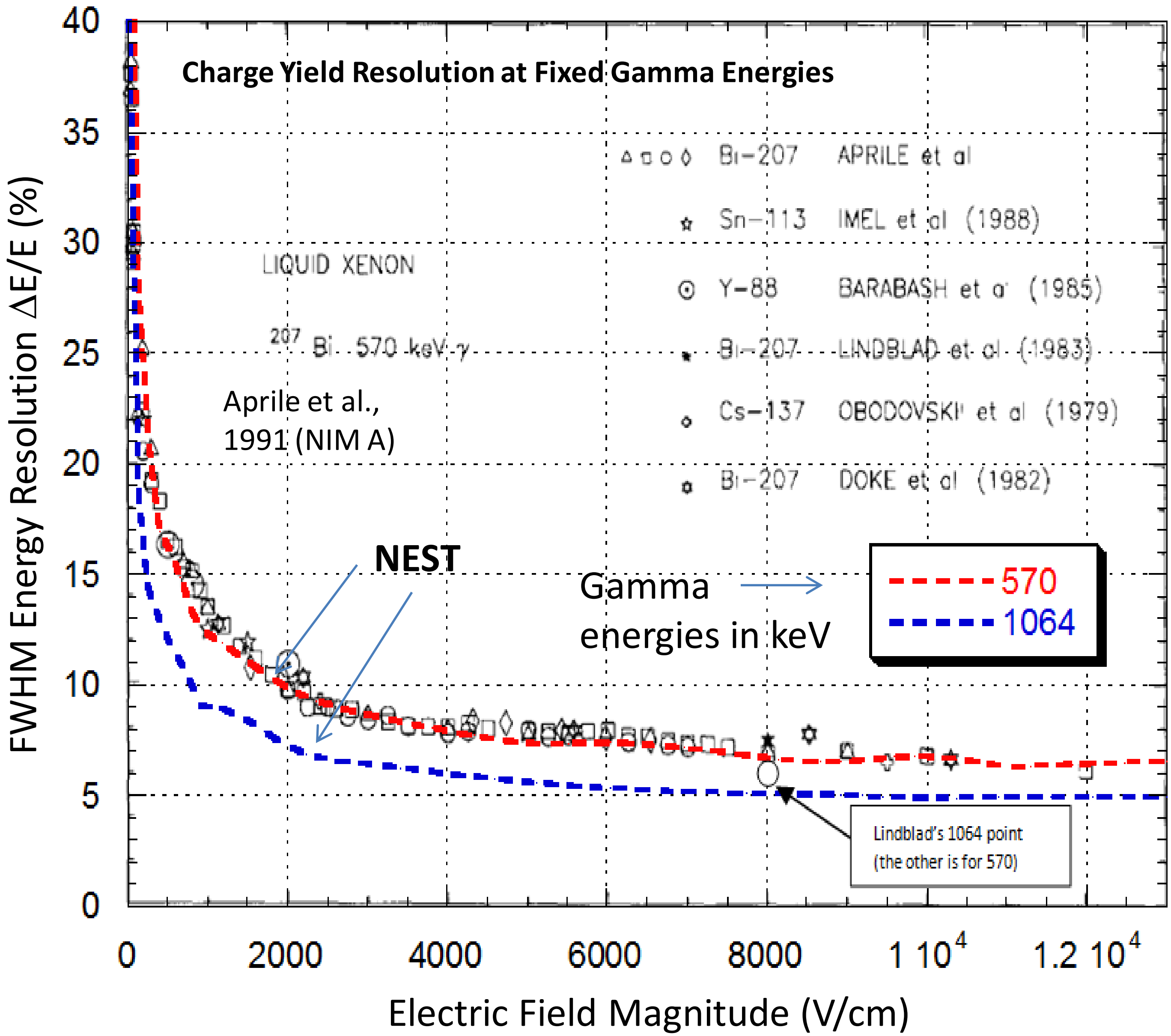


- Regular Fano factor left alone
- Recombination fluctuations have been modeled as worse than binomial, with a 1-sigma of sqrt(F_e*N_e), per interaction site
- Field-dependent but energy-independent

Recombination Fluctuations: S1



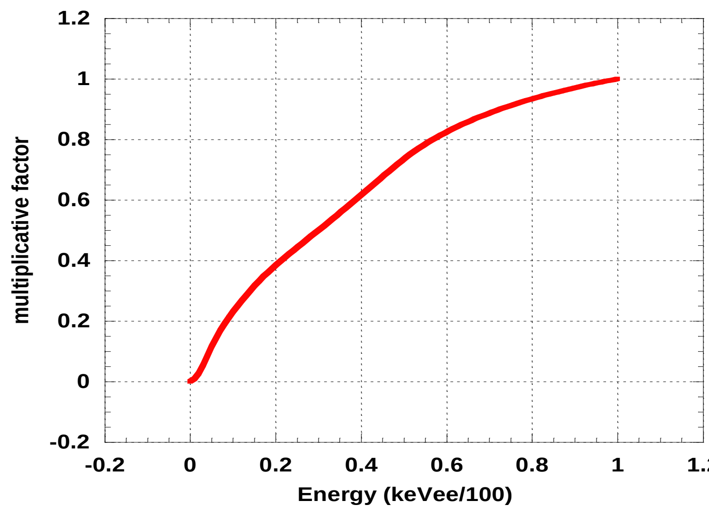
Recombination Fluctuations: Q



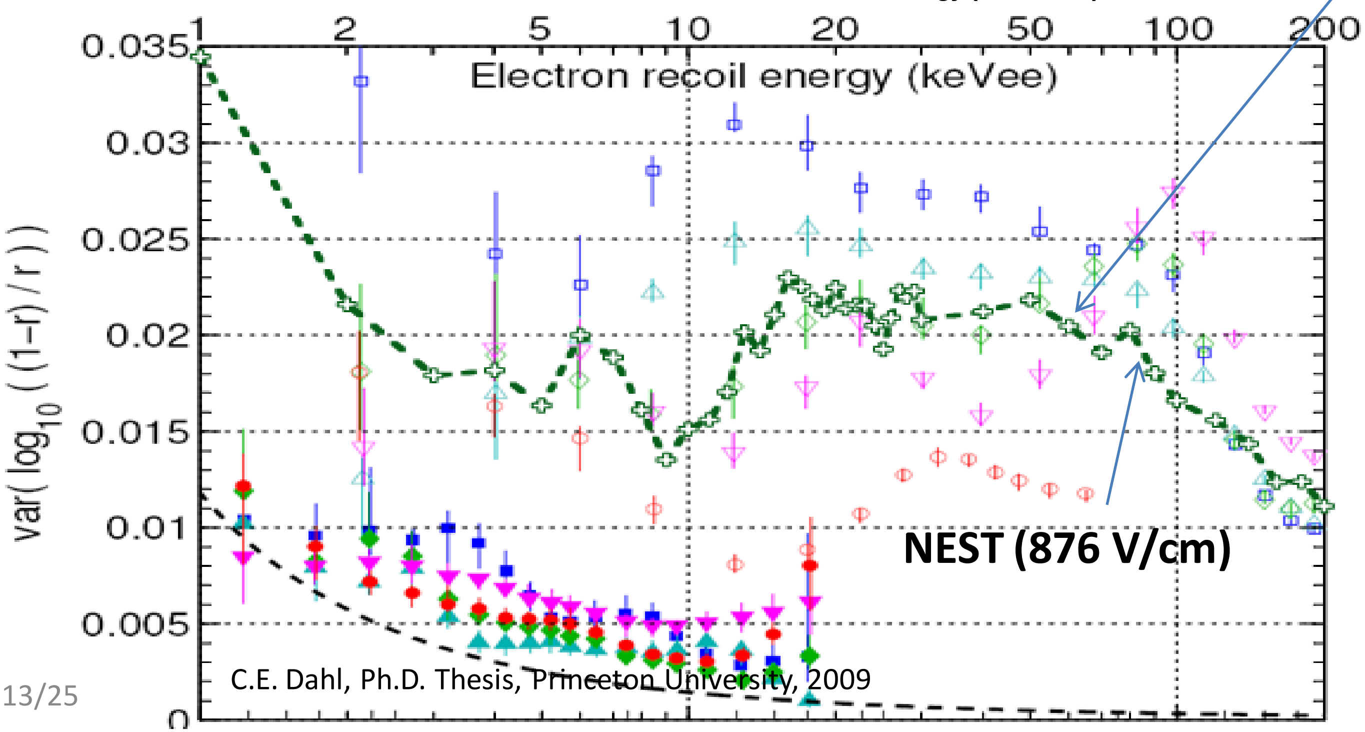
- Showing only ionization channel here
- Unfortunately, best data is for high energy
- Good simulated resolution will allow us to predict the discrimination power of any detector as a function of field and energy

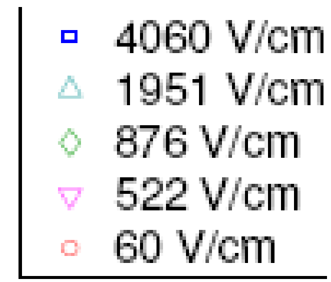
Recombination Fluctuations: Low-E

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



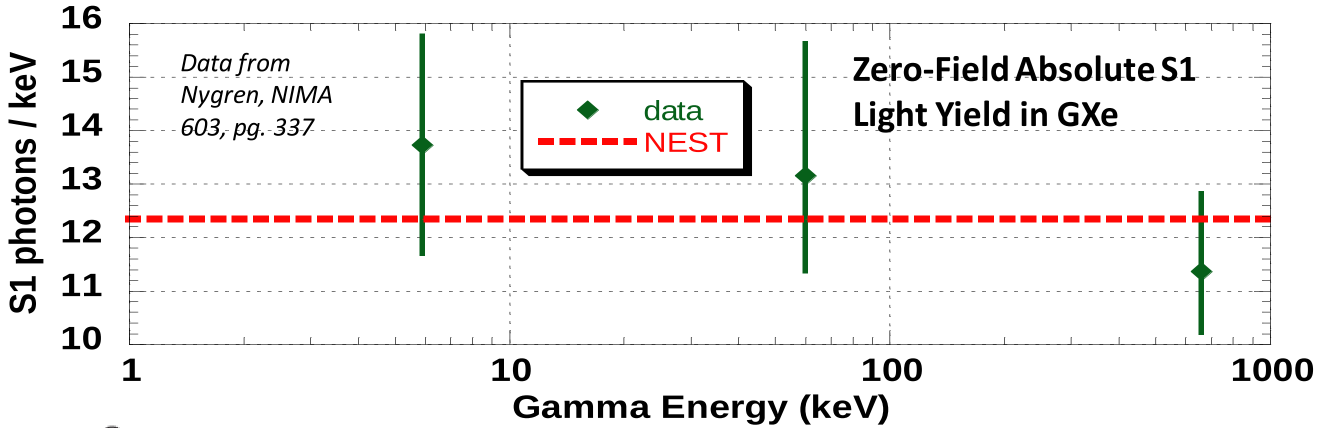
The undulations are at least partially an "emergent property" of NEST, caused by the "battle" between the increasing energy and the increasing variance

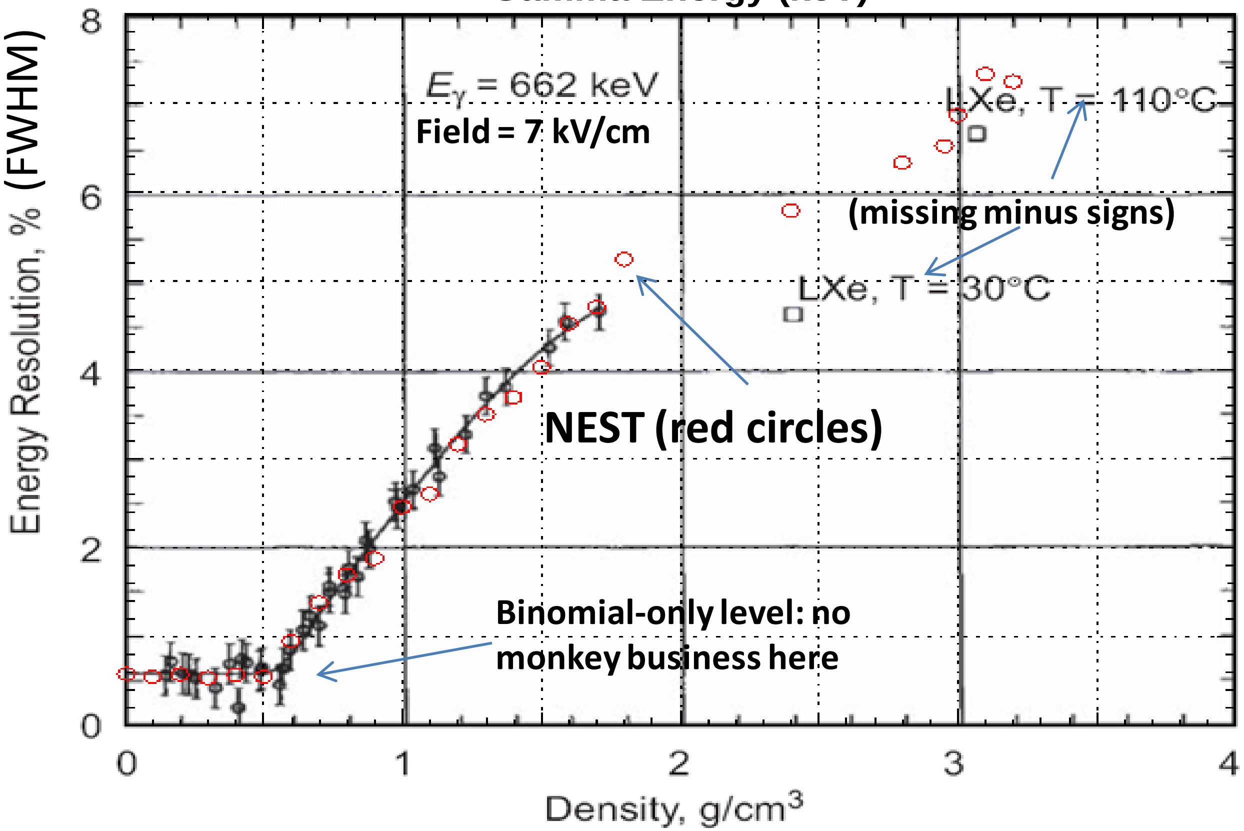




We won't need to have energy resolution as a free parameter in sims anymore, but anticipate it instead, by basing NEST on past data

Gaseous Xenon

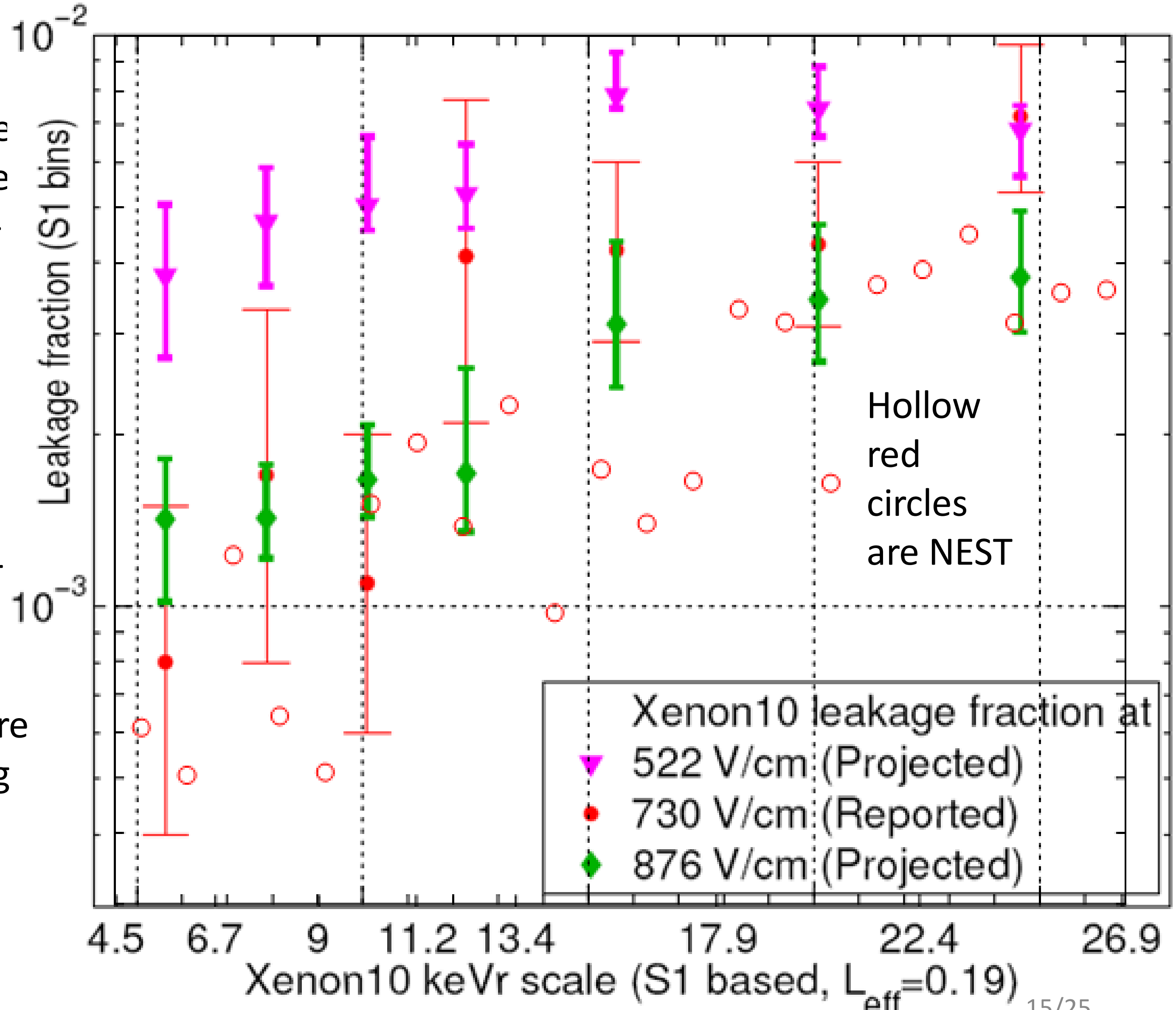




- We can generalize our field-dependent model to be density-dependent, and use it to fit gas data effectively
- The plot at bottom left from Bolotnikov 1997 and Nygren 2009 was considered a bit mysterious: we now have a model to explain it (though it still needs more physical motivation quantitatively)
- NEST has ever-broader applications (double beta decay in this case)

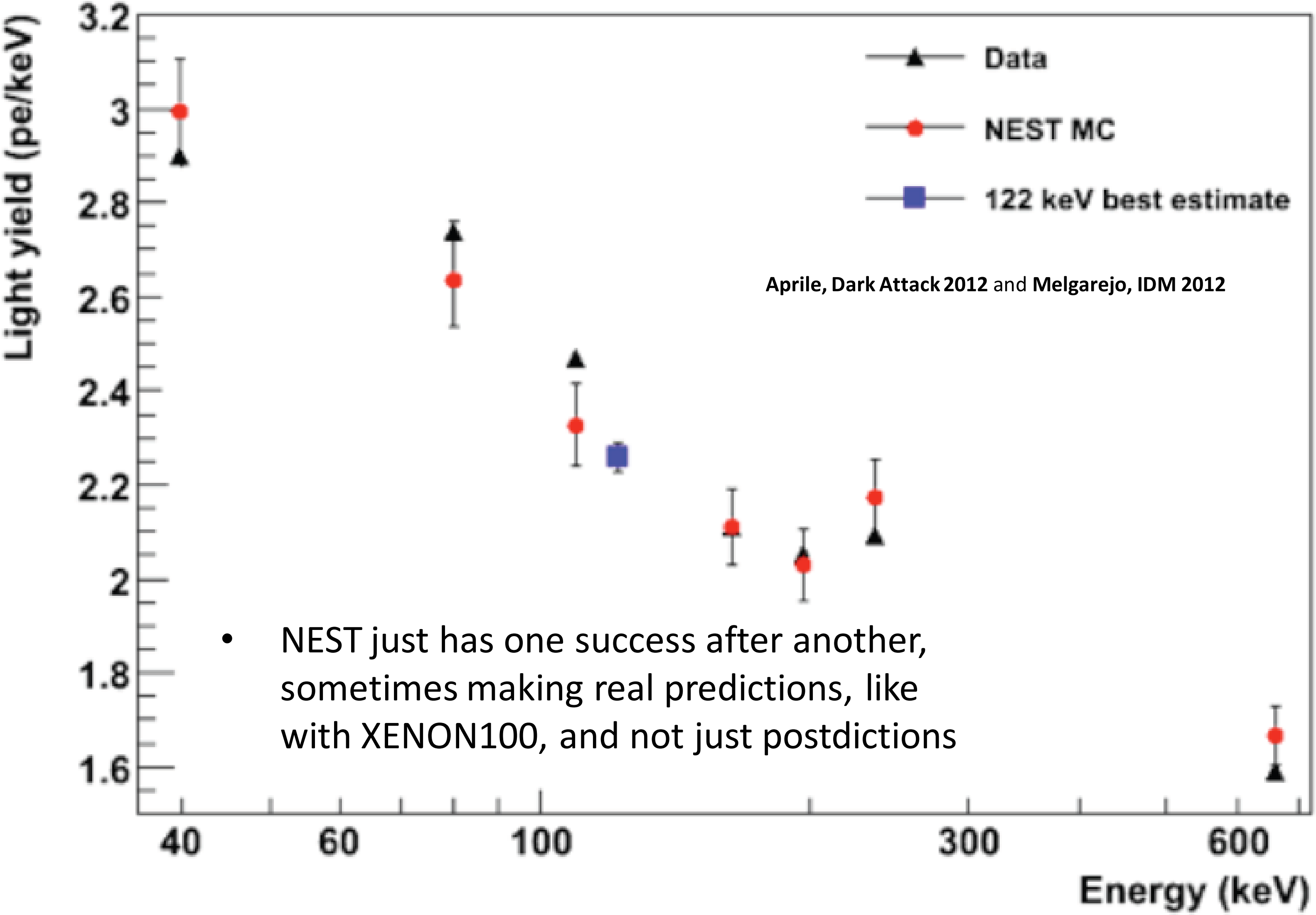
ER vs. NR Discrimination

- After the improvements to the recombination model made to reflect non-Poissonian fluctuations, NEST exhibits the correct behavior for low-E discrimination!
- It should now be possible to use NEST in order to make general predictions for present and future detectors of differing light collection efficiencies and electric fields



Hollow red circles are NEST

Predictive Power Success

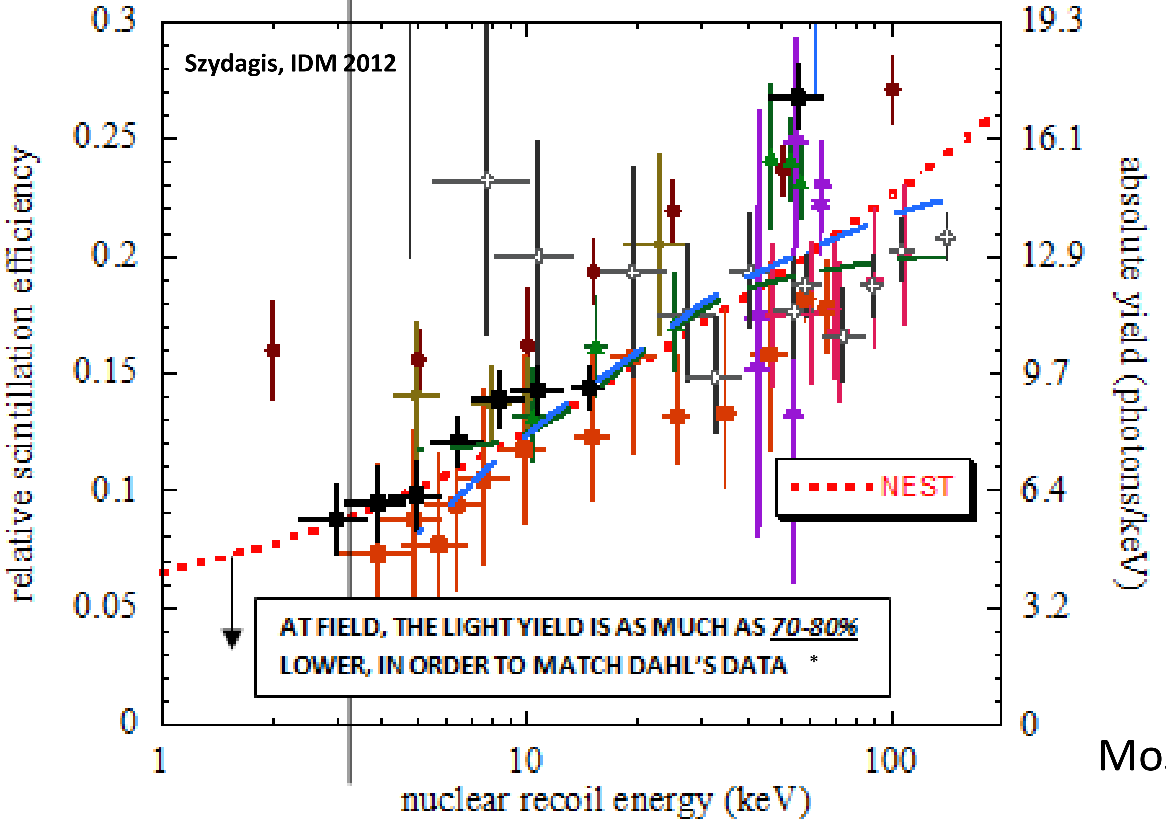


- NEST just has one success after another, sometimes making real predictions, like with XENON100, and not just postdictions

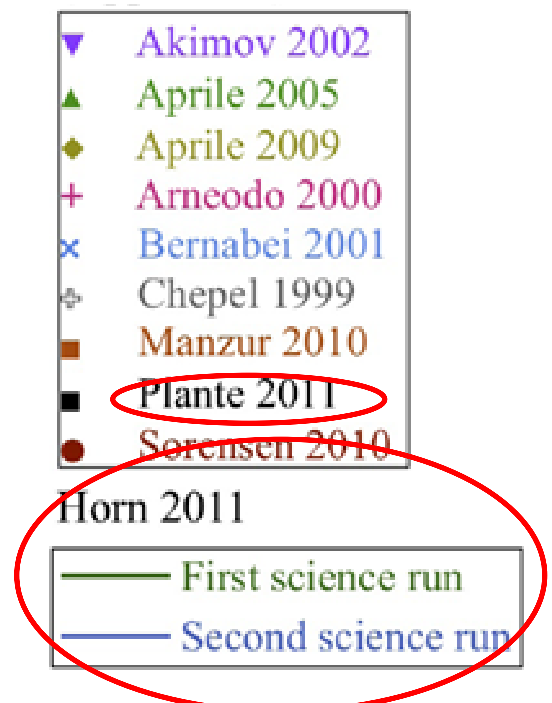
Nuclear Recoil

- Uses Sorensen-Dahl adjusted Lindhard model. NOT a direct fit!
- Uses ER low-E recombination probability and theoretical N_{ex}/N_i

Model goes lower than data,
but it's NOT an extrapolation



Compilation of global data

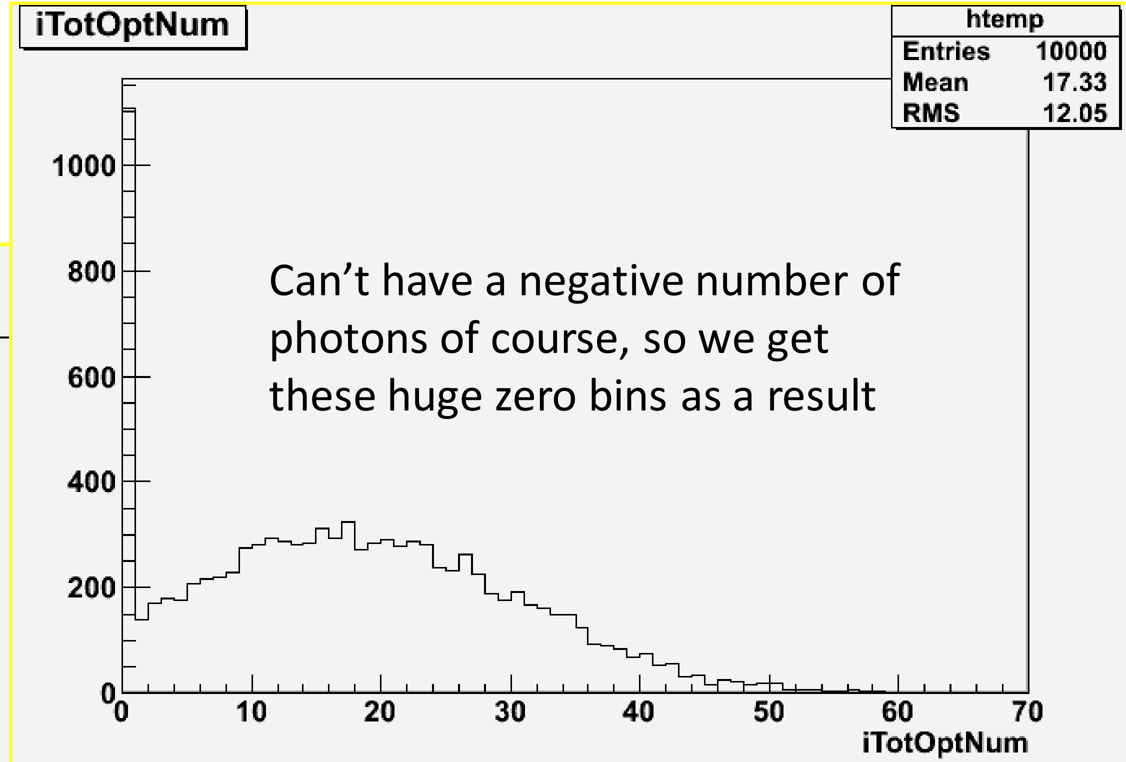


Most recent circled

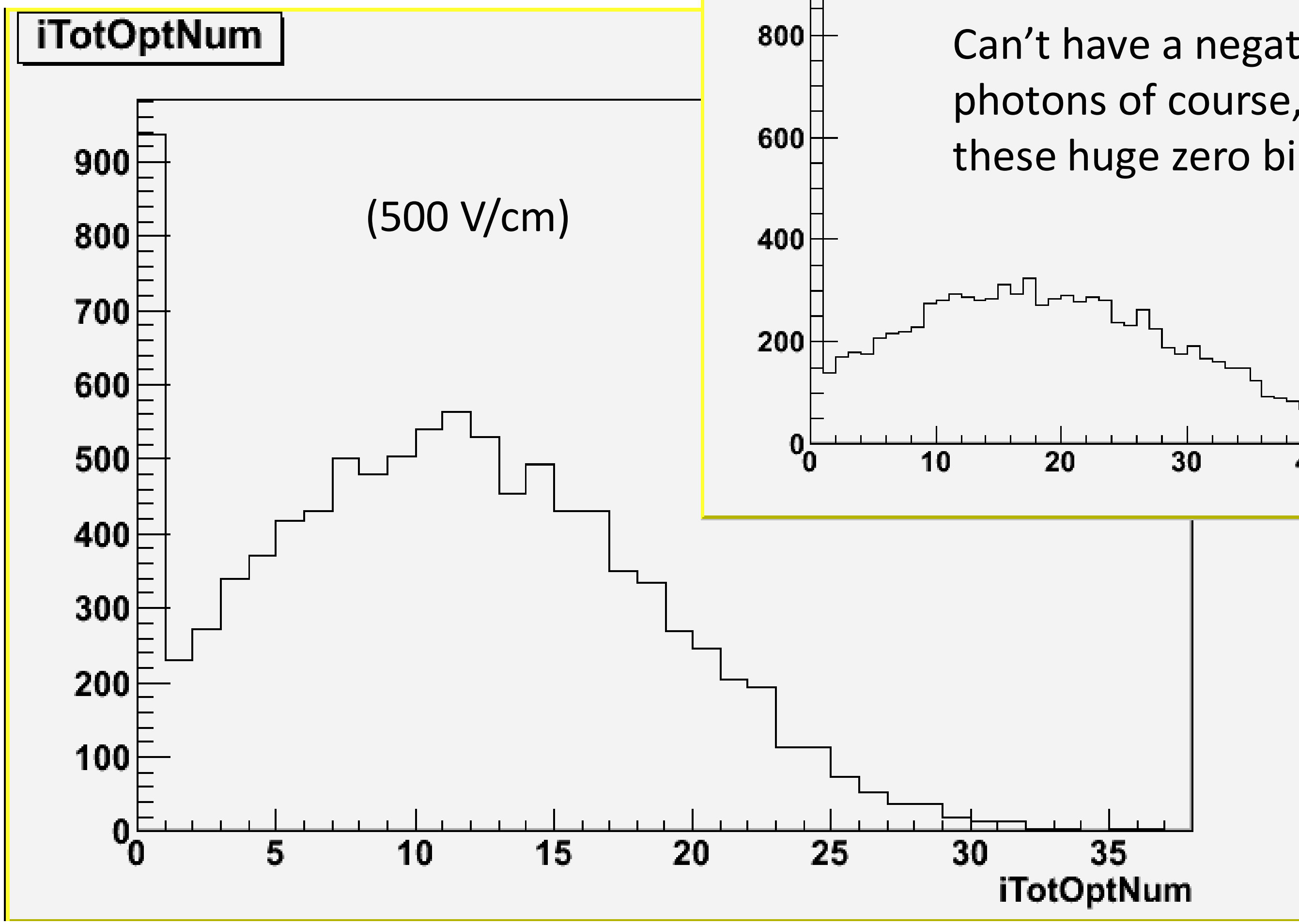
* C.E. Dahl, Ph.D. Thesis, Princeton University, 2009. Paper in preparation...

Non-Gaussianities (Make Tails?)

Absolute numbers of optical photons at low energies: 3 keVnr (below) and 1 keVee (right)



Can’t have a negative number of photons of course, so we get these huge zero bins as a result

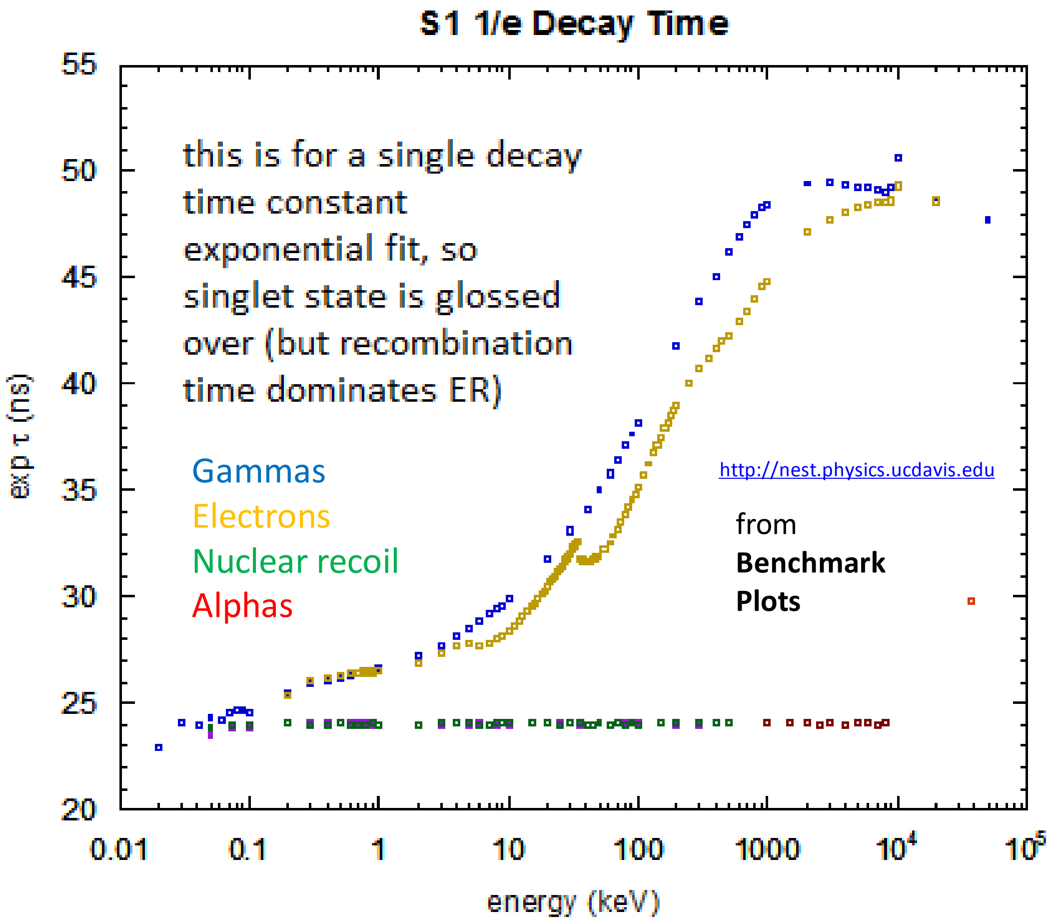


(500 V/cm)

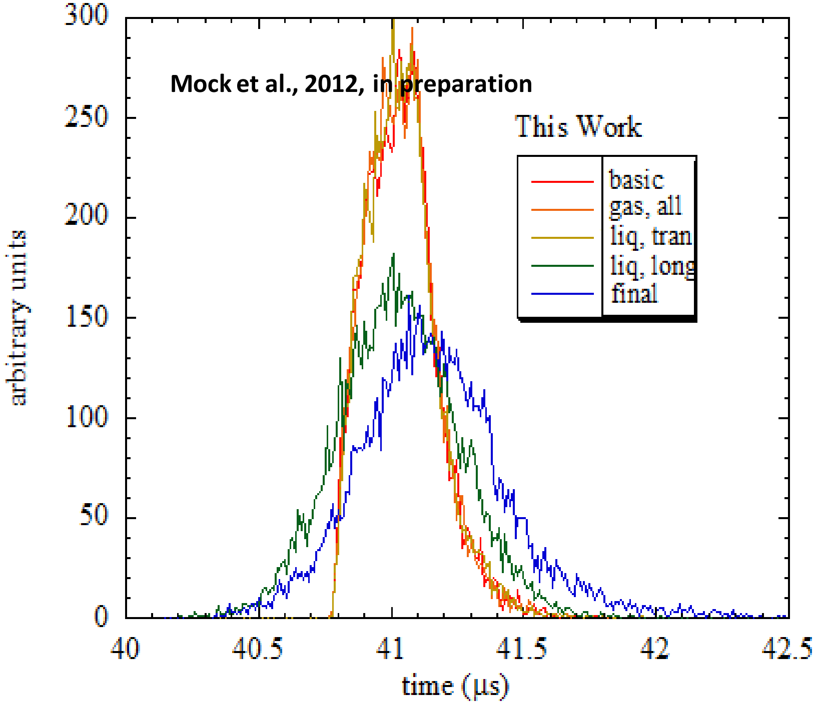
These examples stem from the super-Poissonian fluctuations and don’t include other effects, such as “Gamma-X” events

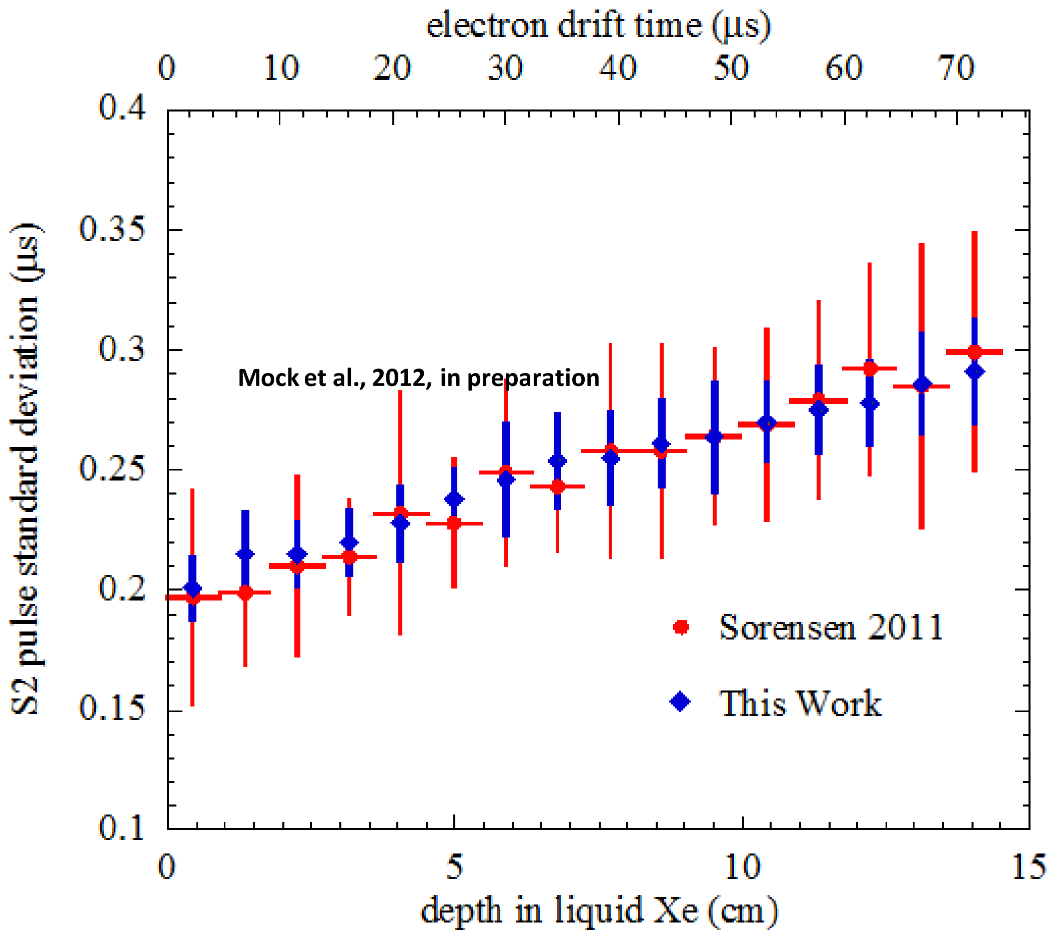
Understanding Pulse Shapes (S1)

- Differences between ER and NR disappear with higher field
- Also disappear at lower energies
- Two exponential time constants corresponding with the triplet and singlet Xe dimer states, but the triplet dominates
- Recombination goes as 1 / time, but time constant not fixed (related to the LET)



Understanding Pulse Shapes (S2)





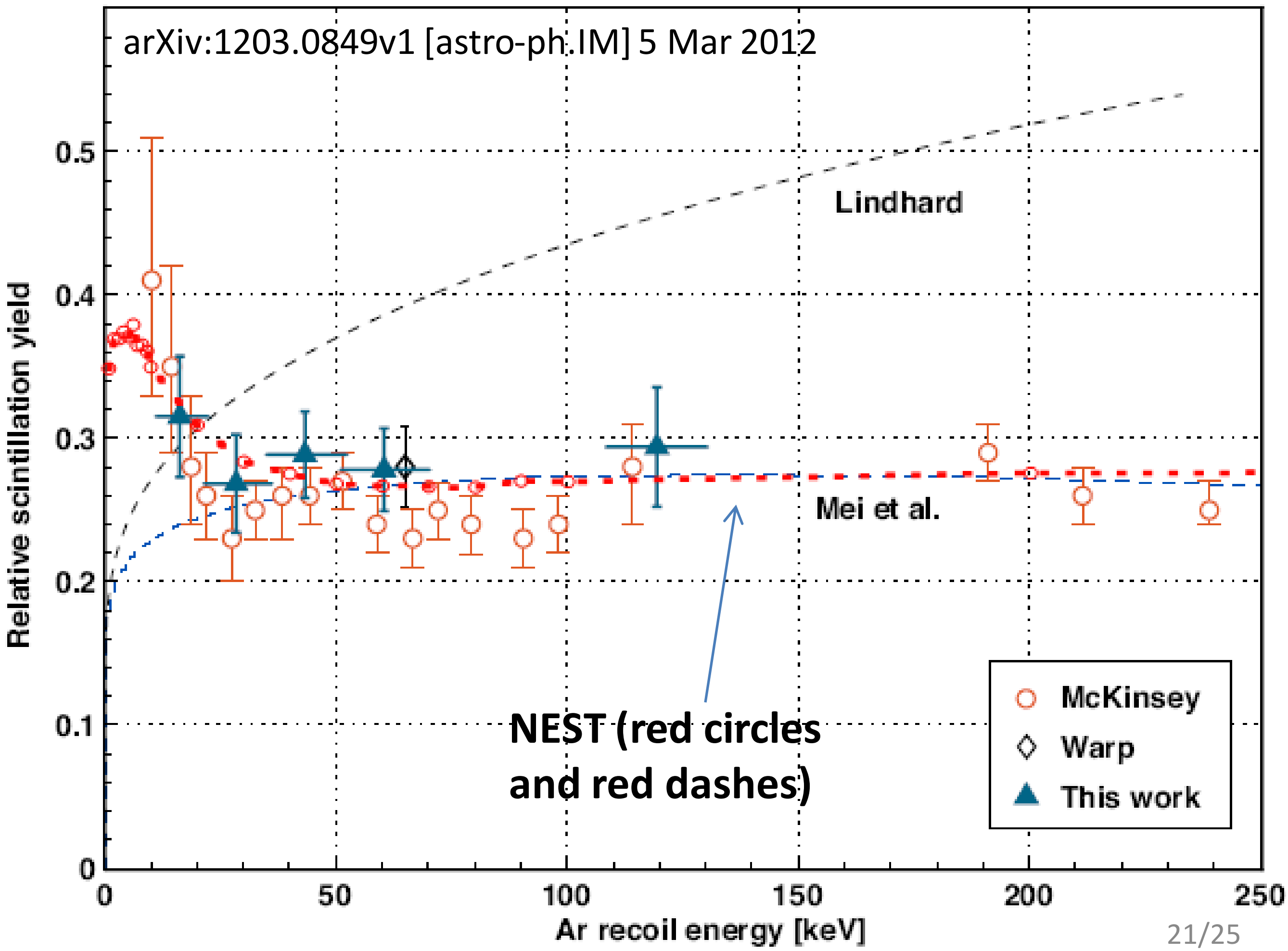
- List of included effects
  - **New G4Particle for drift e-'s**
  - Drift speed (liquid, gas)
  - Triplet, singlet lifetimes
  - Diffusion constants (transverse and longitudinal)
  - Electron trapping time

- Can now reproduce the width of the electroluminescence (S2) gas proportional scintillation pulse as a function of the depth

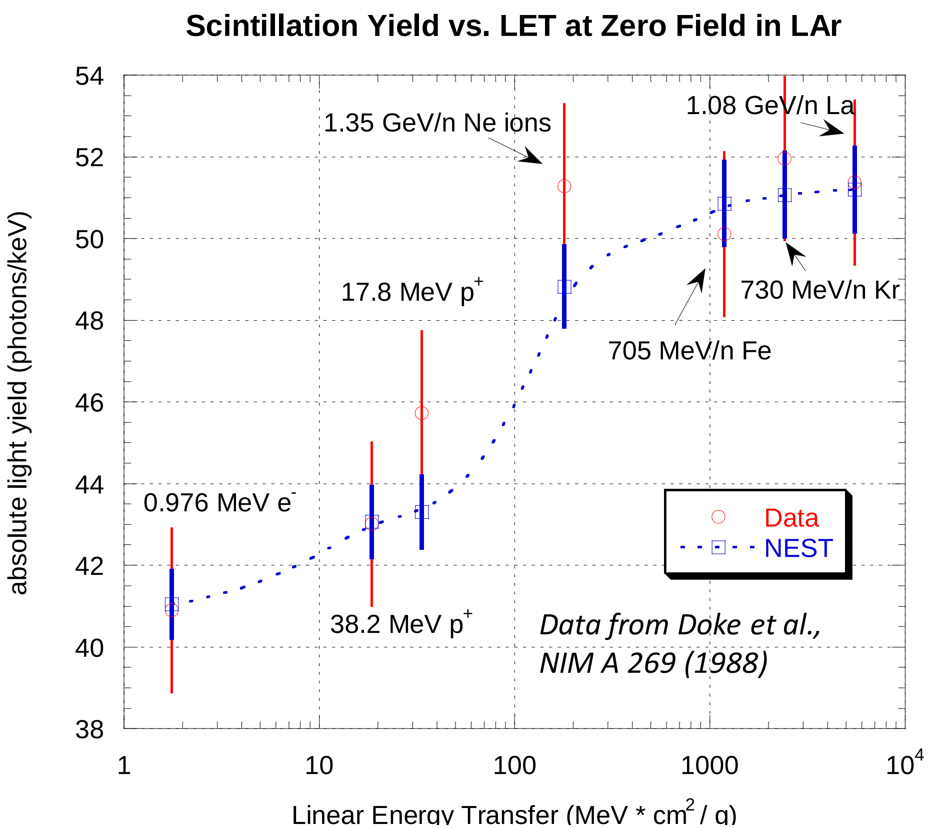
Generalizing This Work to Argon

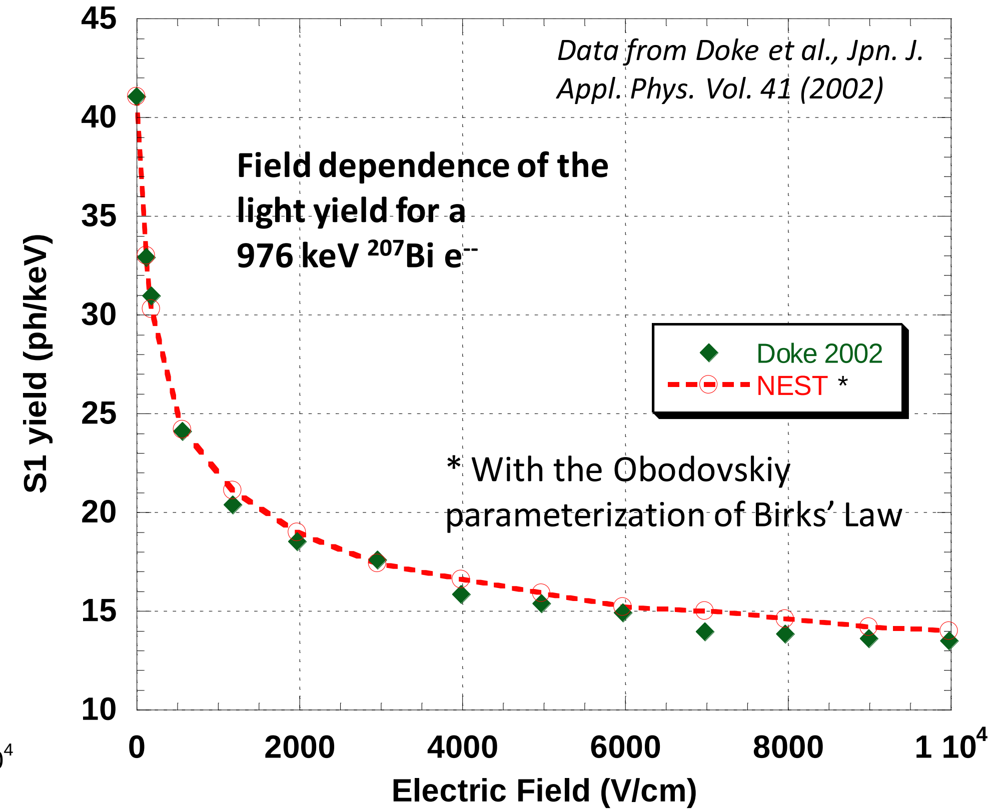
- Relative yield higher than in xenon, because the lighter argon nucleus is more efficient at transferring energy into ionization or excitation
- The NEST model is the only one that can explain the apparently higher yield at lower energies, appealing to cross-section enhancement (work of Bezrukov 2011 on LXe)

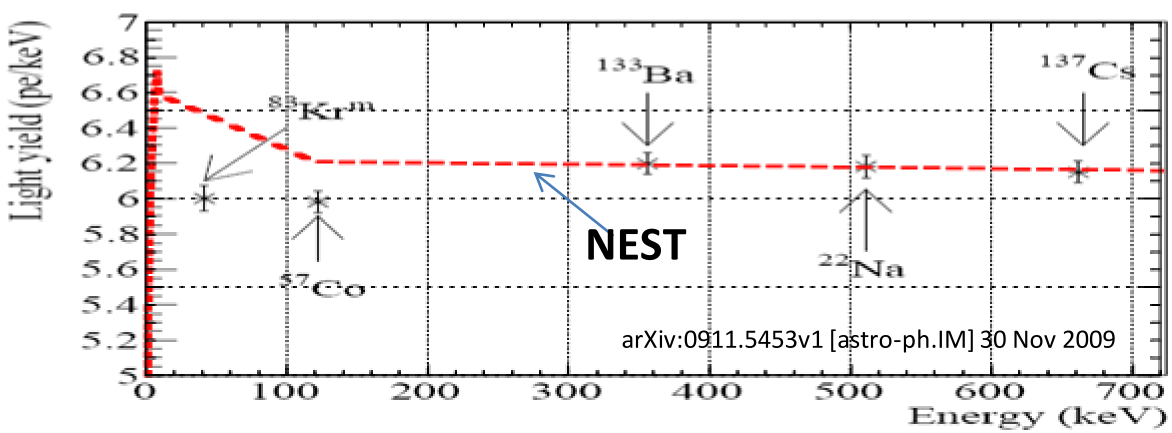
The NEST curve is generated assuming a flat L-factor. The downward curve at low energy is caused by the recombination probability falling from necessity, in the Thomas-Imel recombination model



Generalizing This Work to Argon

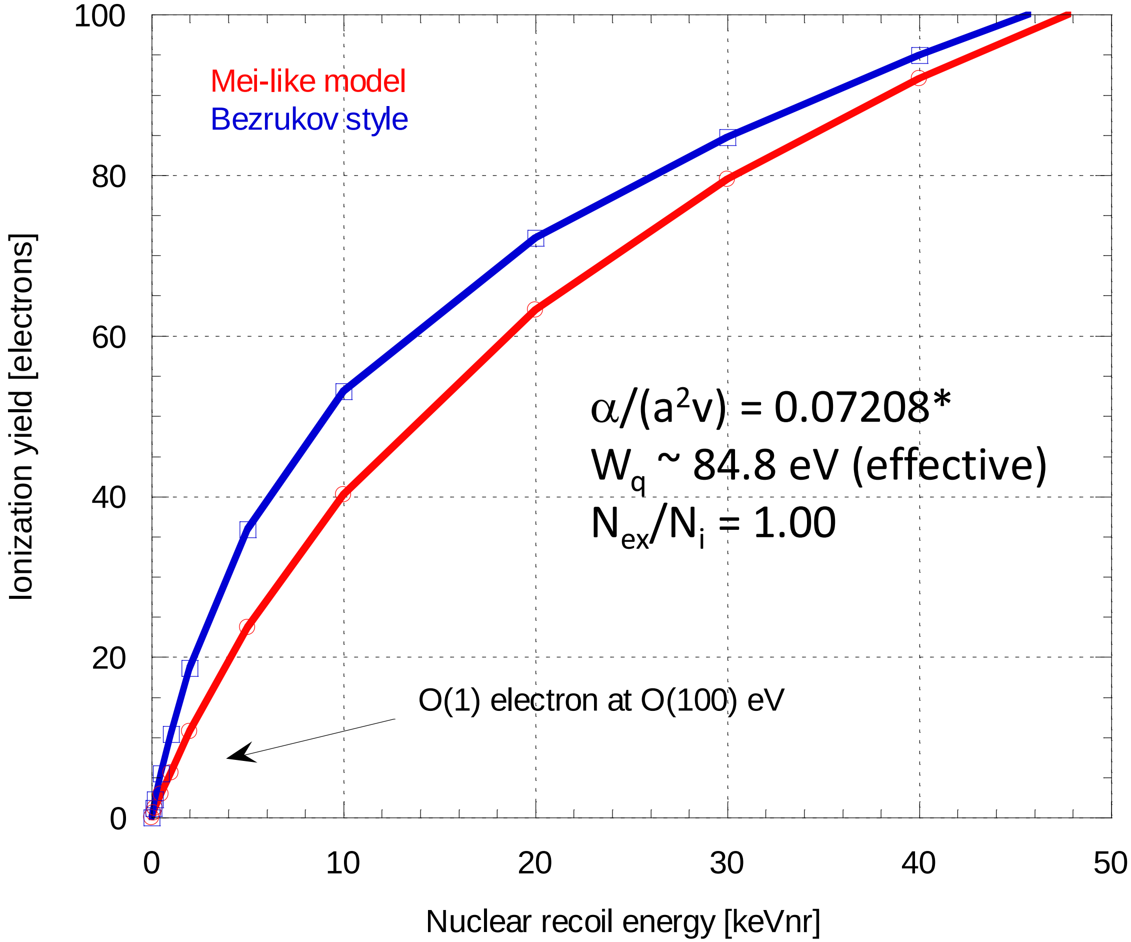






- NEST even works out to the multi-MeV to GeV regime (applicable to LBNE), and out to O(10) kV/cm (PANDA-X)
- With xenon fully simulated, we're just now scratching the surface of liquid argon

Generalizing to Ar: LLNL Applications



- Prediction set from NEST at left for nuclear recoil charge yield. Data can disambiguate different models
- Post-diction for electron recoil not shown (redundant): Samuele and I made the same calculations

*Samuele's number. My back of the envelope yielded O(0.1)

Summary

- The widths of the log10(S2/S1) bands are now more properly modeled than before, with supra-Poissonian fluctuations
- Work on Xe in NEST (for both liquid and gas) is rapidly nearing FULL completion, culminating in being able to model the ER vs. NR discrimination ability in liquid, and the changing energy resolution between liquid and gas: NEST has matured a lot!
- You can now input your background model and get your expected “misidentification-as-WIMP” rate for your detector more accurately than with past simulations
- Maybe first appearance of simulated non-Gaussian tails in LXe
- Work on Ar and other elements is starting to ramp up, and NEST is already starting to tackle the LAr field-dependent yield for electron recoils, and the ever-tricky L-factor for NR, but long way to go before looking at discrimination in argon

References

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

  M. Szydagis et al., NEST: A Comprehensive Model For Scintillation Yield in Liquid Xenon 2011 **JINST** 6 P10002. arxiv:1106.1613

  (Our paper does not have everything covered in this talk or already available in the code, but more papers are on the way....)