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

http://nest.physics.ucdavis.edu

Matthew Szydagis
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

LBNL Brown Bag Talk, Berkeley, CA, Thursday 08/23/2012

The People of the NEST Team

UC Davis and LLNL
A small but passionate group of individuals who love their work

Faculty
Mani Tripathi

Physicists
Kareem Kazkaz

Postdocs
Matthew Szydagis*

Undergraduate
Students
Francisco Baltazar
Nichole Barry
Adalyn Fyhrie

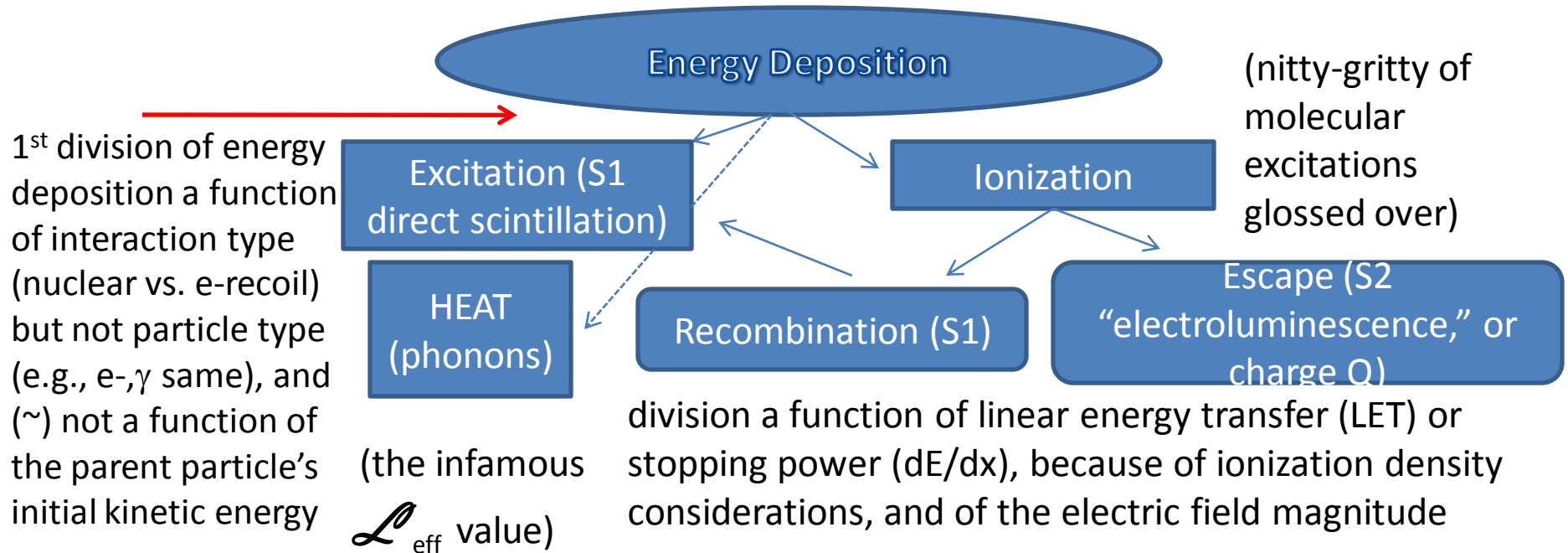Graduate Students
Jeremy Mock
Nick Walsh
Mike Woods

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, … both 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

Energy Deposition

(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

Excitation (S1 direct scintillation)

Ionization

HEAT (phonons)

Recombination (S1)

Escape (S2 "electroluminescence," or charge Q)

(the infamous $\mathcal{L}_{eff}$ 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
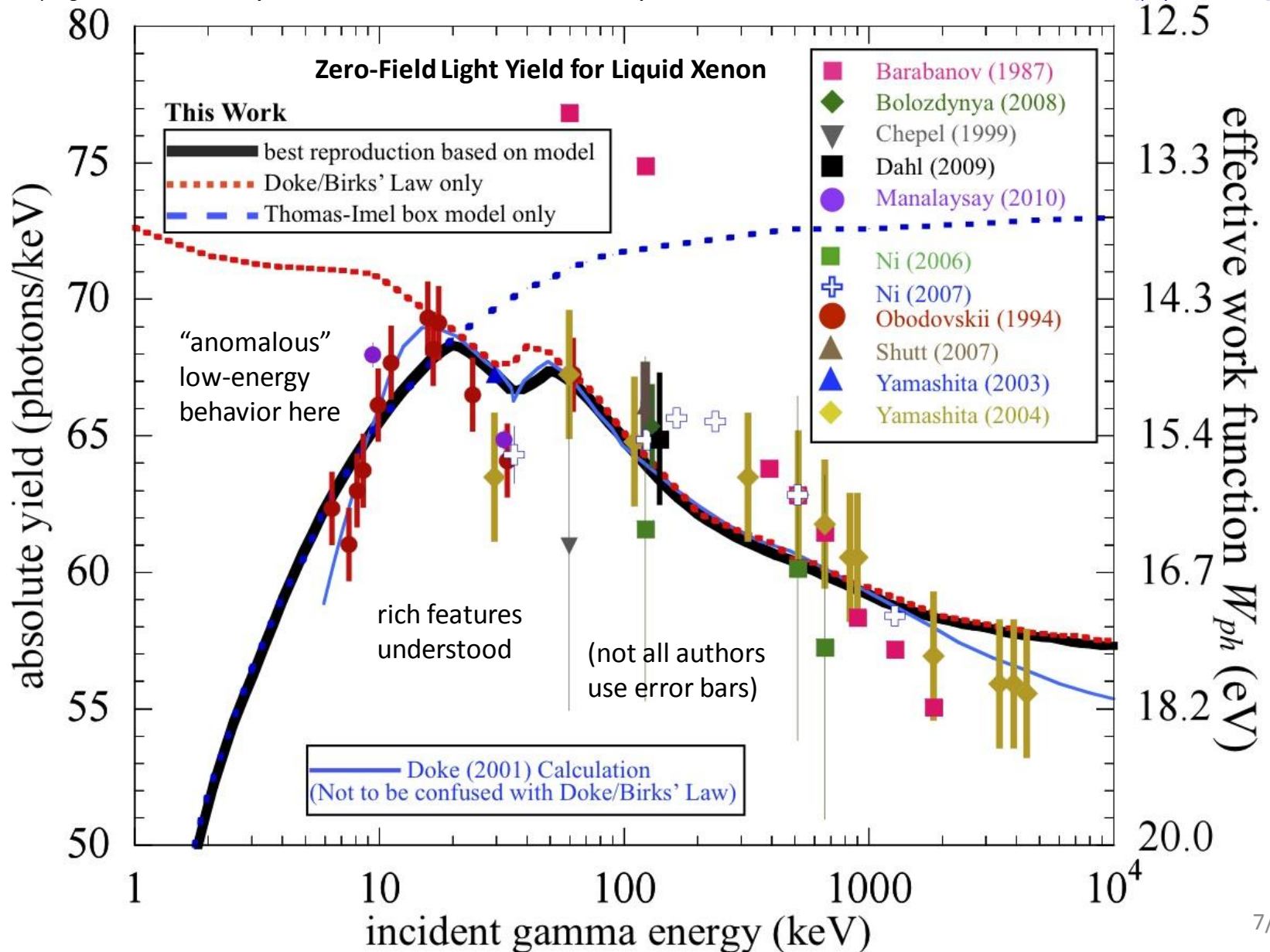
- Heat loss for nuclear recoils (Lindhard effect), while electron recoils relatively easier to deal with

- Start simple: no exotic energy loss mechanisms (like "bi-excitonic" collisions). Explains the data?
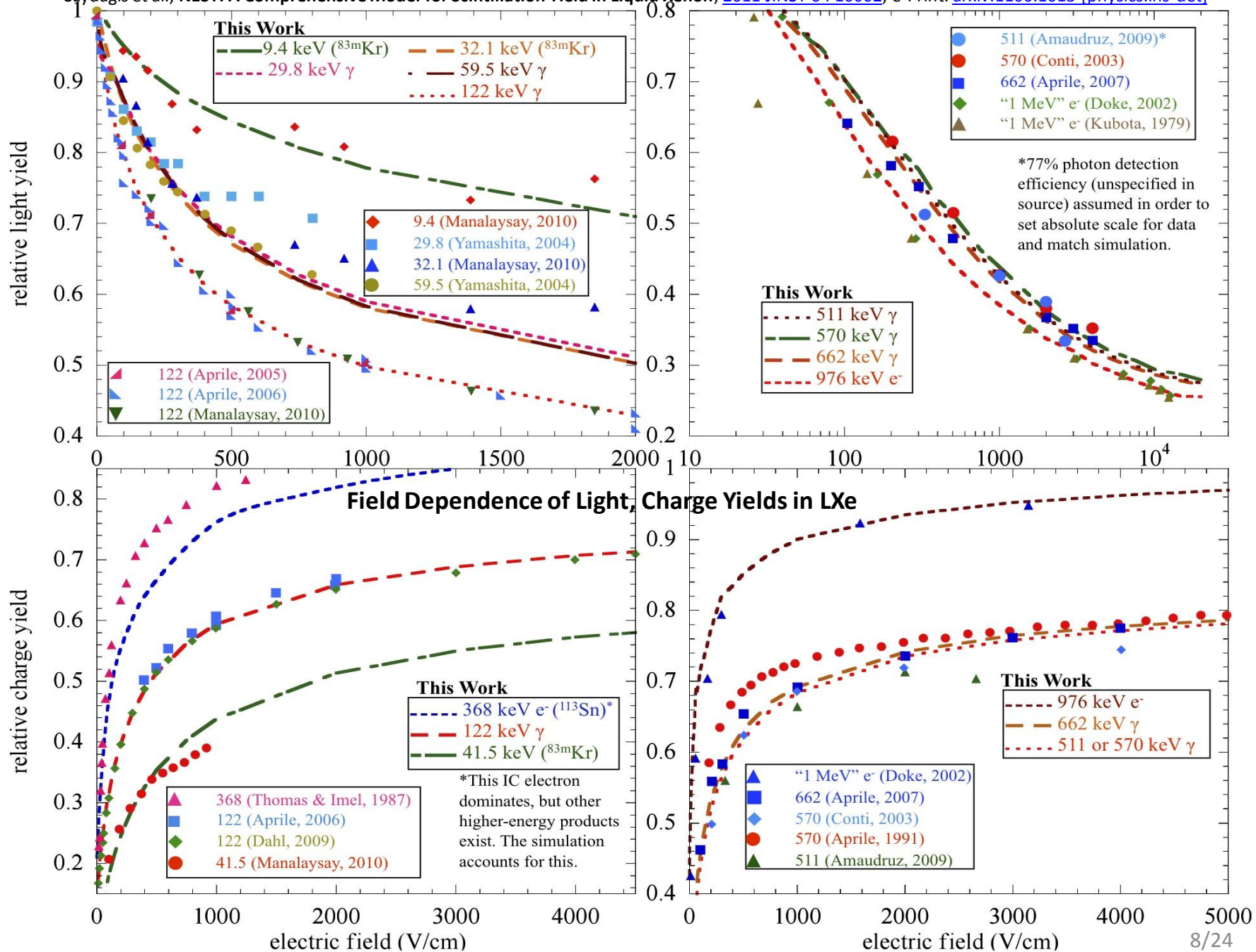
Basic Physics Principles

- 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 $\quad N_q = (N_{e-} + N_{\gamma}) = E_{dep} / W$

  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
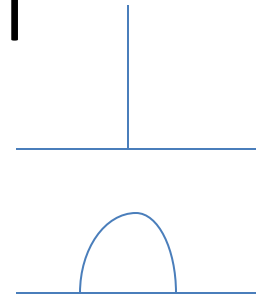
Putting it All Together to Predict Yield

Zero-Field Light Yield for Liquid Xenon

"anomalous" low-energy behavior here

rich features understood

(not all authors use error bars)

This Work
- best reproduction based on model
- Doke/Birks' Law only
- Thomas-Imel box model only

- Barabanov (1987)
- Bolozdynya (2008)
- Chepel (1999)
- Dahl (2009)
- Manalaysay (2010)
- Ni (2006)
- Ni (2007)
- Obodovskii (1994)
- Shutt (2007)
- Yamashita (2003)
- Yamashita (2004)

Doke (2001) Calculation
(Not to be confused with Doke/Birks' Law)

Field Dependence of Light, Charge Yields in LXe

Top-left panel legends:

This Work
- 9.4 keV (^{83m}Kr)
- 32.1 keV (^{83m}Kr)
- 29.8 keV γ
- 59.5 keV γ
- 122 keV γ

- 9.4 (Manalaysay, 2010)
- 29.8 (Yamashita, 2004)
- 32.1 (Manalaysay, 2010)
- 59.5 (Yamashita, 2004)

- 122 (Aprile, 2005)
- 122 (Aprile, 2006)
- 122 (Manalaysay, 2010)

Top-right panel legends:

- 511 (Amaudruz, 2009)*
- 570 (Conti, 2003)
- 662 (Aprile, 2007)
- "1 MeV" e⁻ (Doke, 2002)
- "1 MeV" e⁻ (Kubota, 1979)

*77% photon detection efficiency (unspecified in source) assumed in order to set absolute scale for data and match simulation.

This Work
- 511 keV γ
- 570 keV γ
- 662 keV γ
- 976 keV e⁻

Bottom-left panel legends:

This Work
- 368 keV e⁻ (^{113}Sn)*
- 122 keV γ
- 41.5 keV (^{83m}Kr)

*This IC electron dominates, but other higher-energy products exist. The simulation accounts for this.

- 368 (Thomas & Imel, 1987)
- 122 (Aprile, 2006)
- 122 (Dahl, 2009)
- 41.5 (Manalaysay, 2010)

Bottom-right panel legends:

This Work
- 976 keV e⁻
- 662 keV γ
- 511 or 570 keV γ

- "1 MeV" e⁻ (Doke, 2002)
- 662 (Aprile, 2007)
- 570 (Conti, 2003)
- 570 (Aprile, 1991)
- 511 (Amaudruz, 2009)

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)
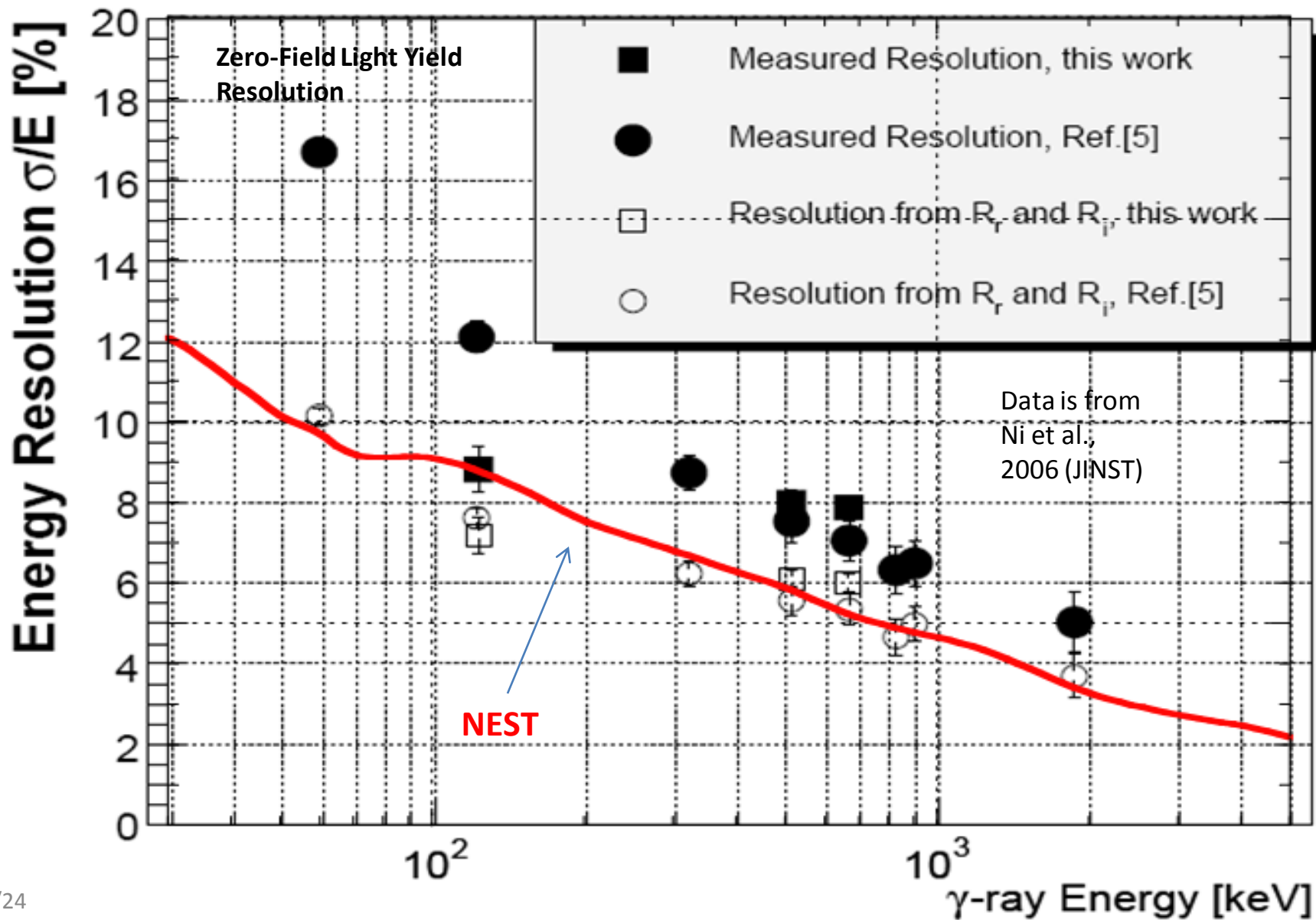- Angle of particle track with respect to electric field vector not yet included

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

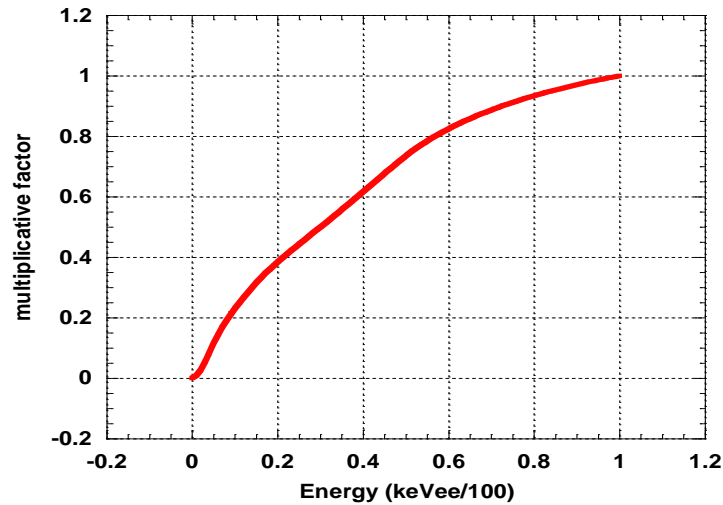# Recombination Fluctuations: S1
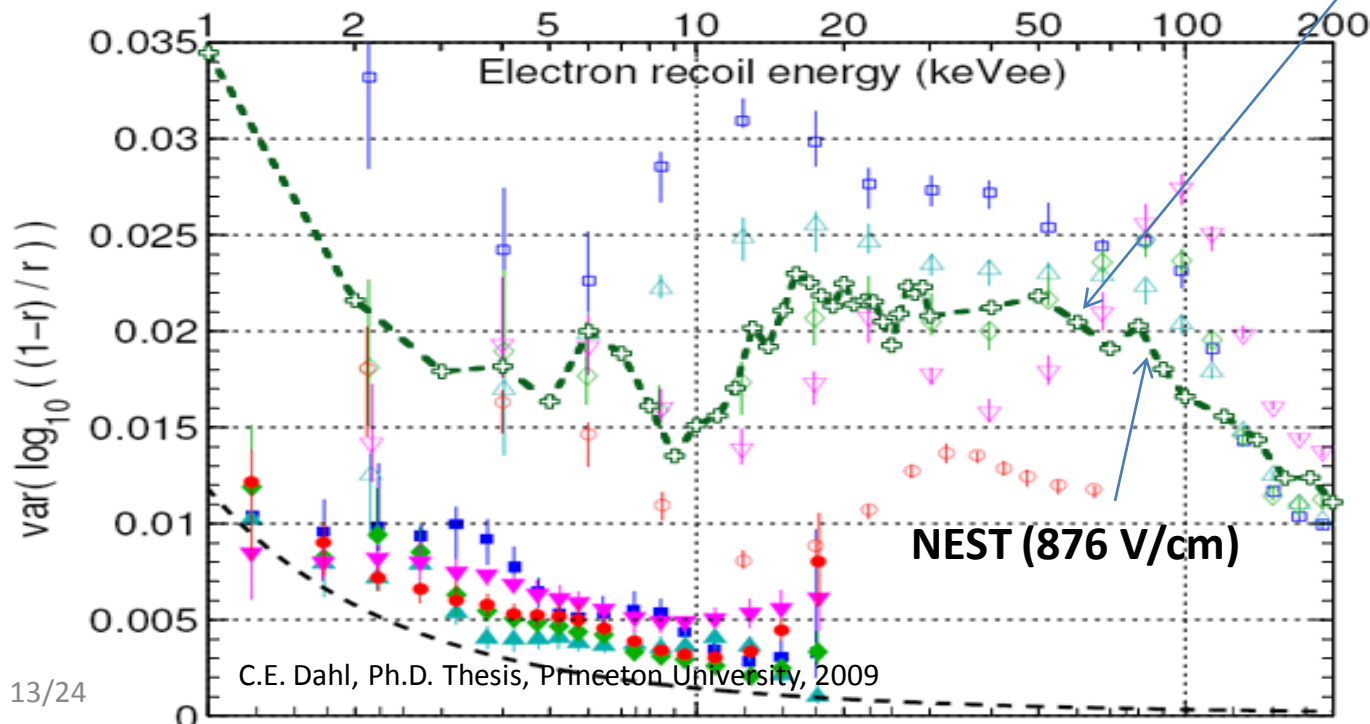
Recombination Fluctuations: Q

Charge Yield Resolution at Fixed Gamma Energies

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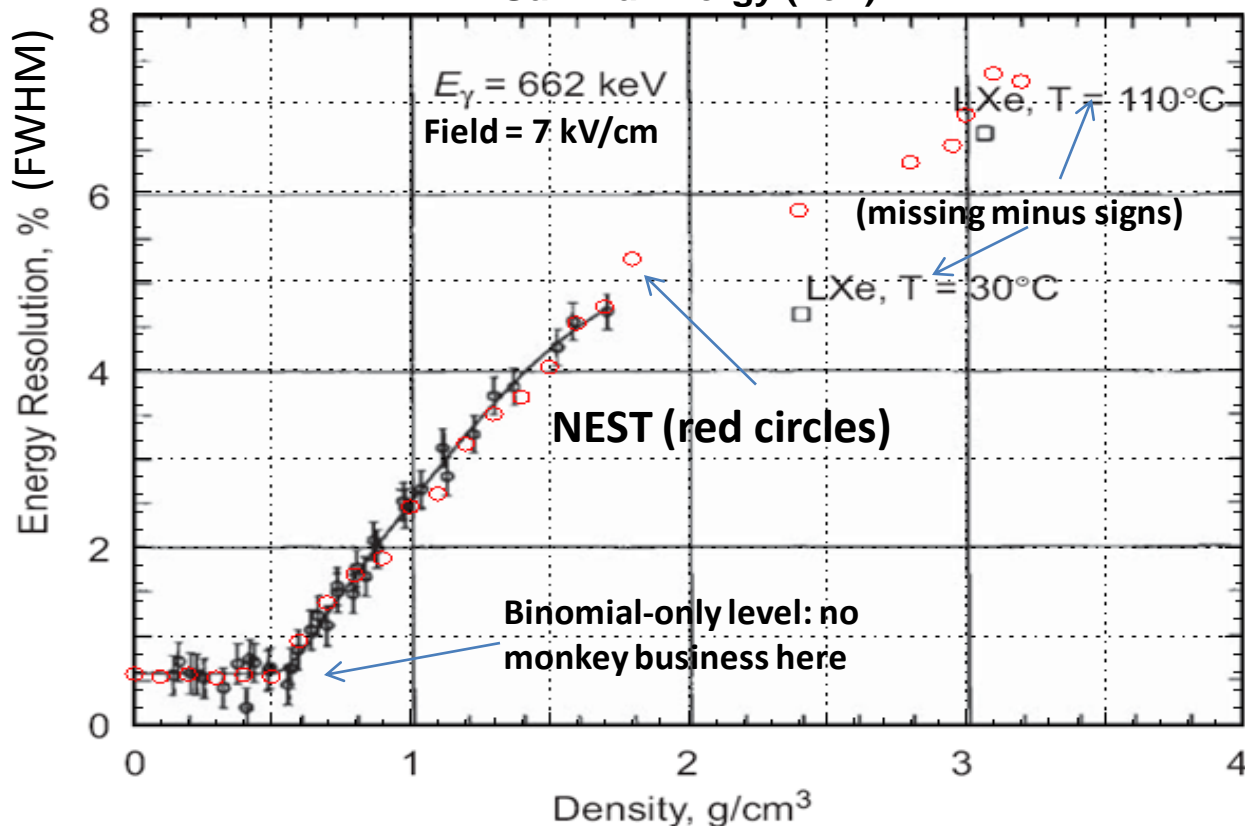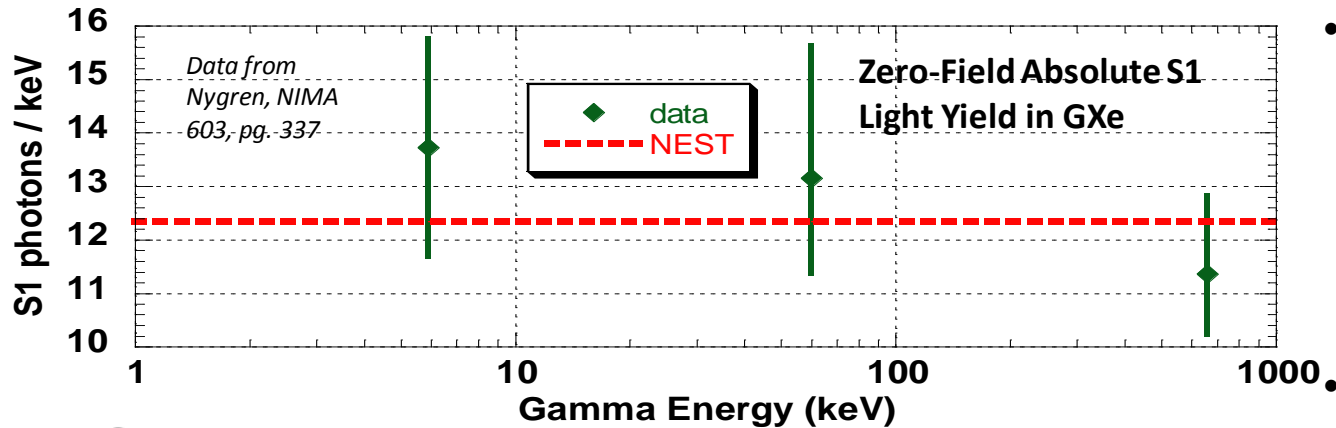
The undulations are at least partially an "emergent property" of NEST, caused by the "battle" between the increasing energy and the increasing variance

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

NEST (876 V/cm)
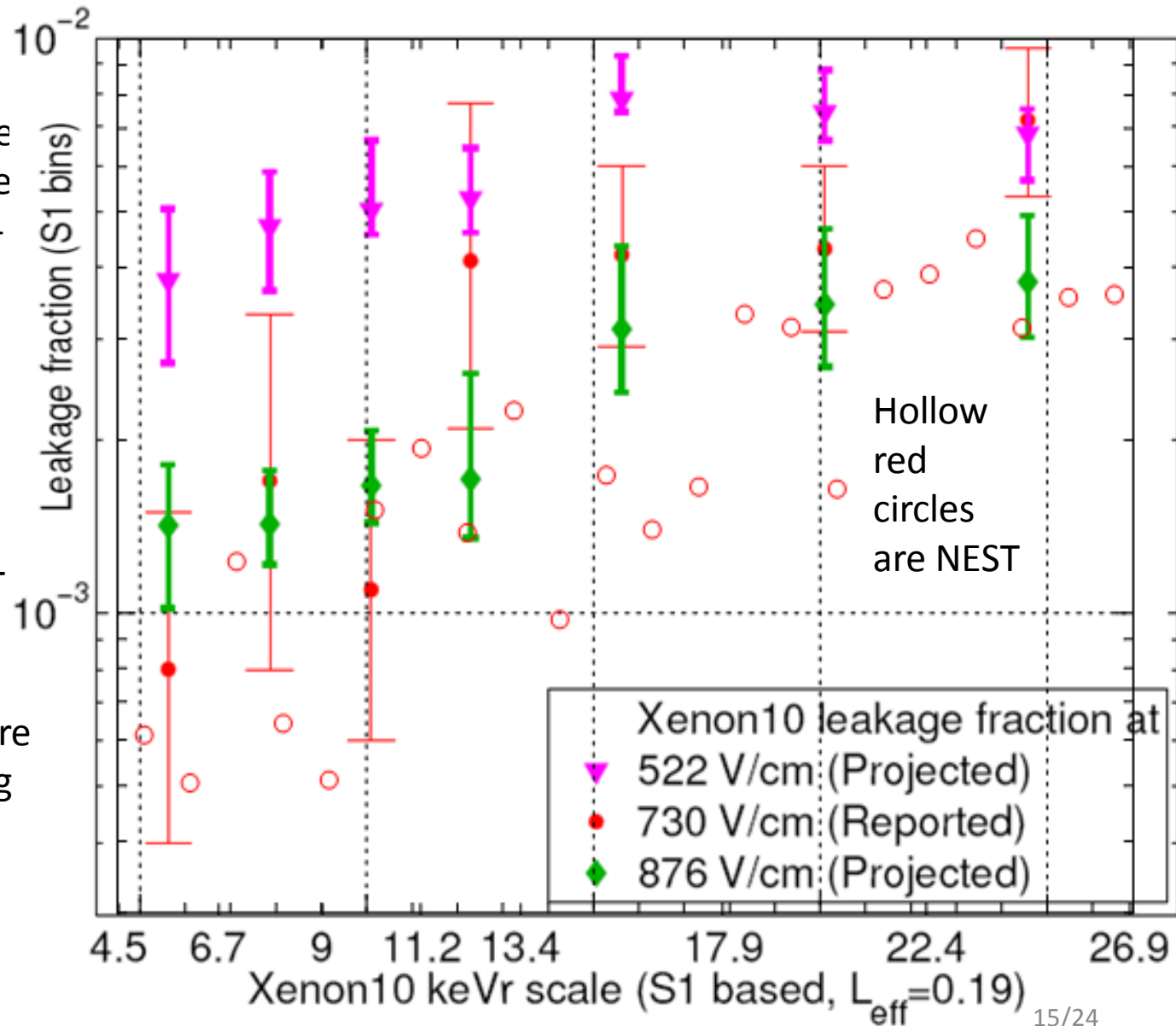
4060 V/cm
1951 V/cm
876 V/cm
522 V/cm
60 V/cm

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

Gaseous Xenon

Data from Nygren, NIMA 603, pg. 337

Zero-Field Absolute S1 Light Yield in GXe

data
NEST

(top plot axes: S1 photons / keV vs Gamma Energy (keV))

$E_\gamma = 662$ keV
Field = 7 kV/cm

LXe, T = 110°C
(missing minus signs)
LXe, T = 30°C

NEST (red circles)

Binomial-only level: no monkey business here

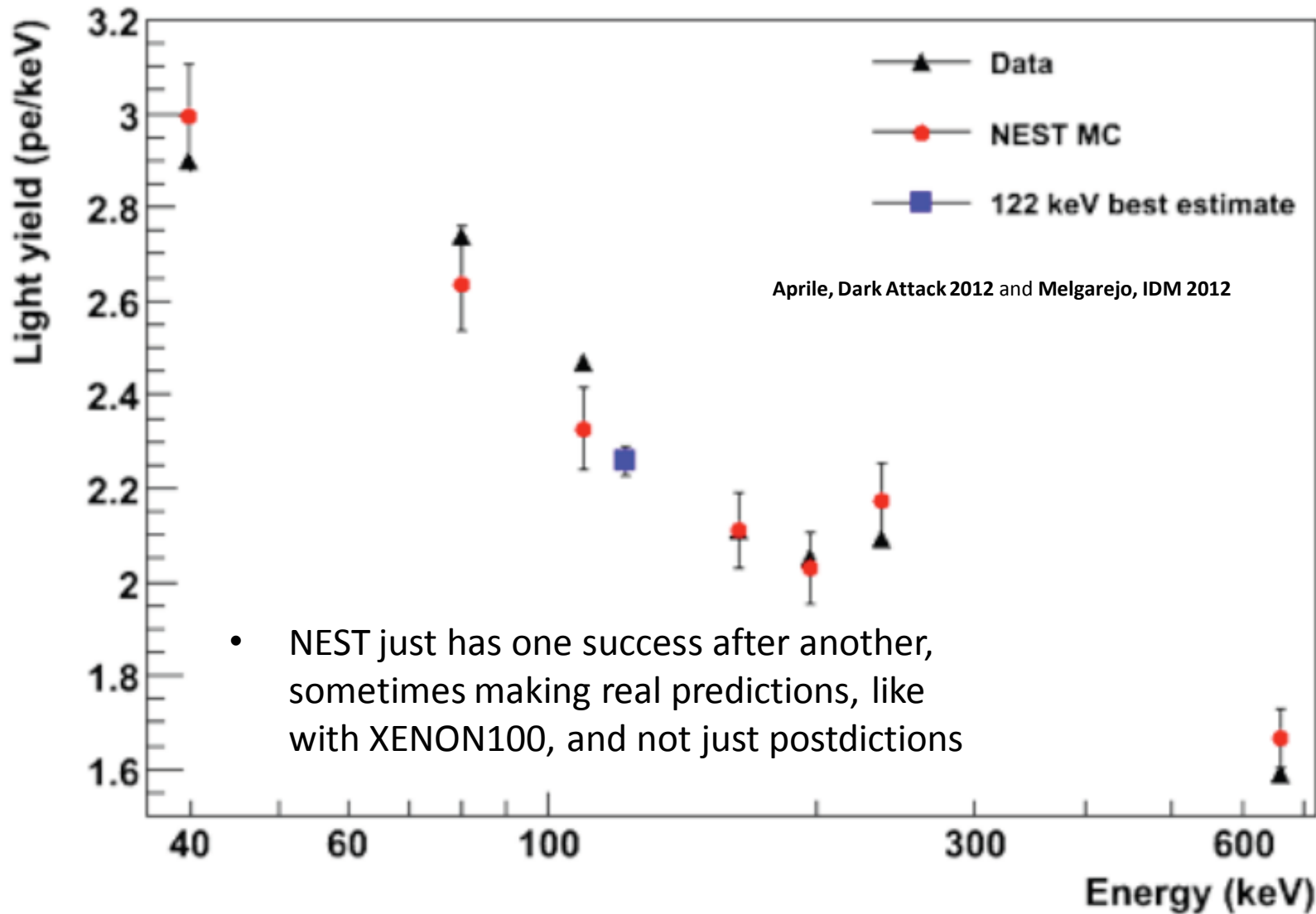(bottom plot axes: Energy Resolution, % (FWHM) vs Density, g/cm^3)

- 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
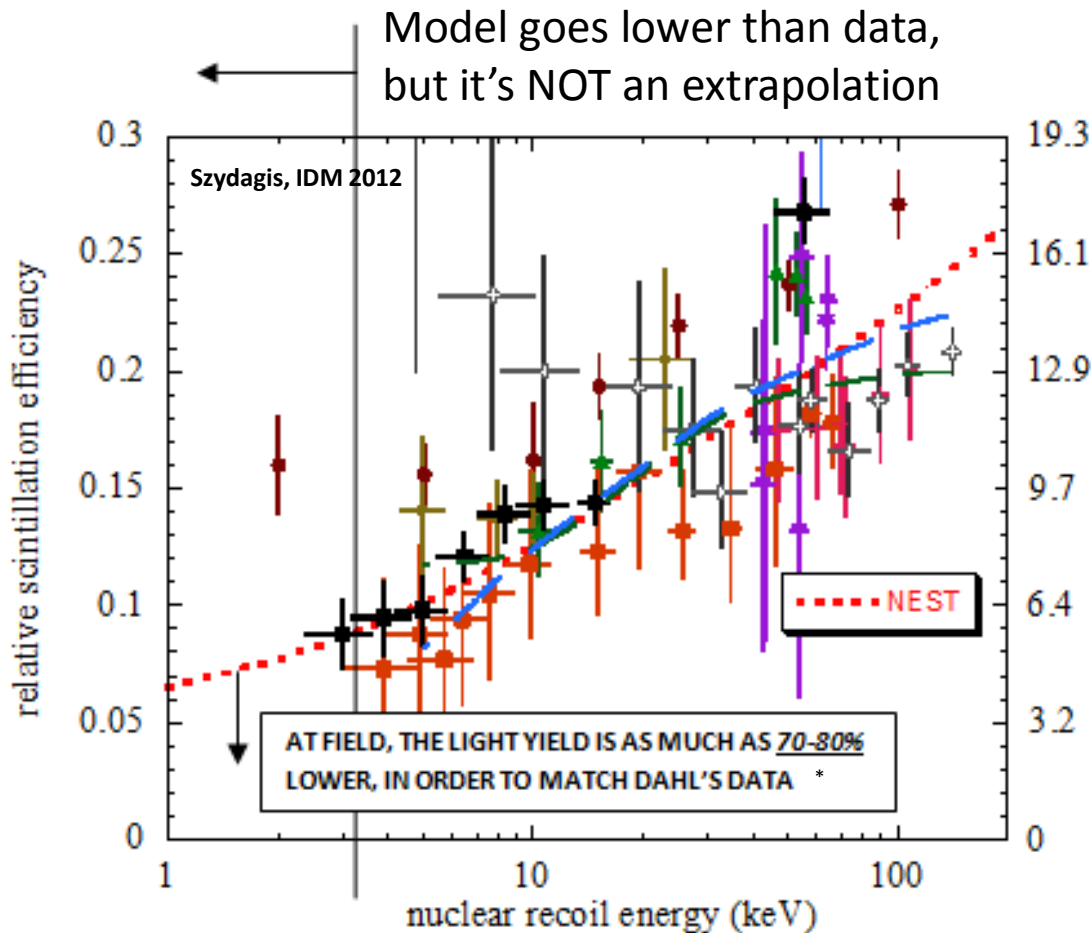
Hollow red circles are NEST

Legend:

Xenon10 leakage fraction at
- 522 V/cm (Projected)
- 730 V/cm (Reported)
- 876 V/cm (Projected)

Y-axis: Leakage fraction (S1 bins)

X-axis: Xenon10 keVr scale (S1 based, $L_{eff}=0.19$)

Predictive Power Success

Aprile, Dark Attack 2012 and Melgarejo, IDM 2012

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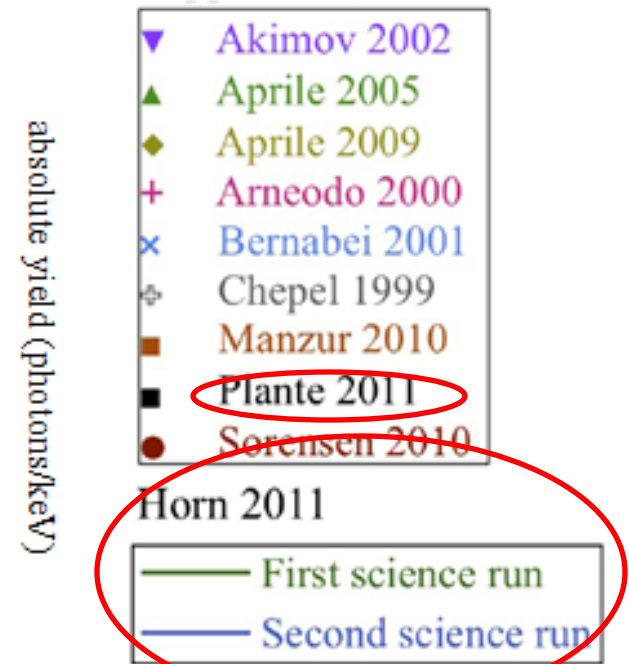
Nuclear Recoil

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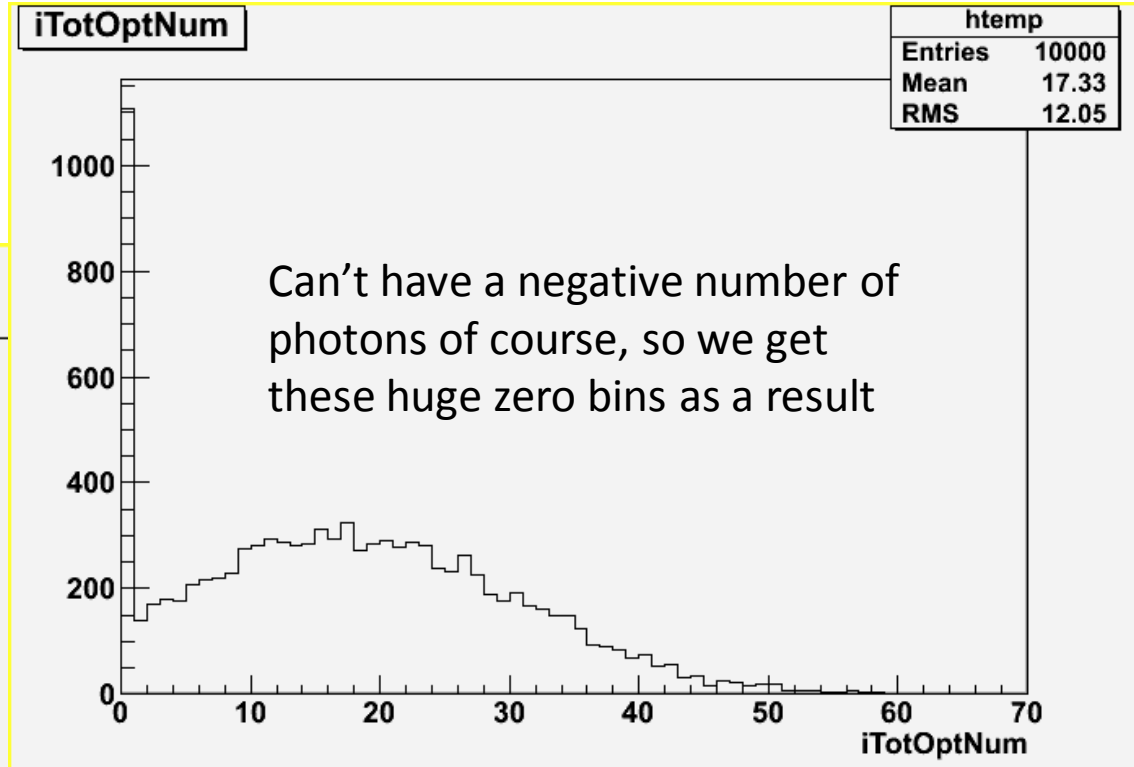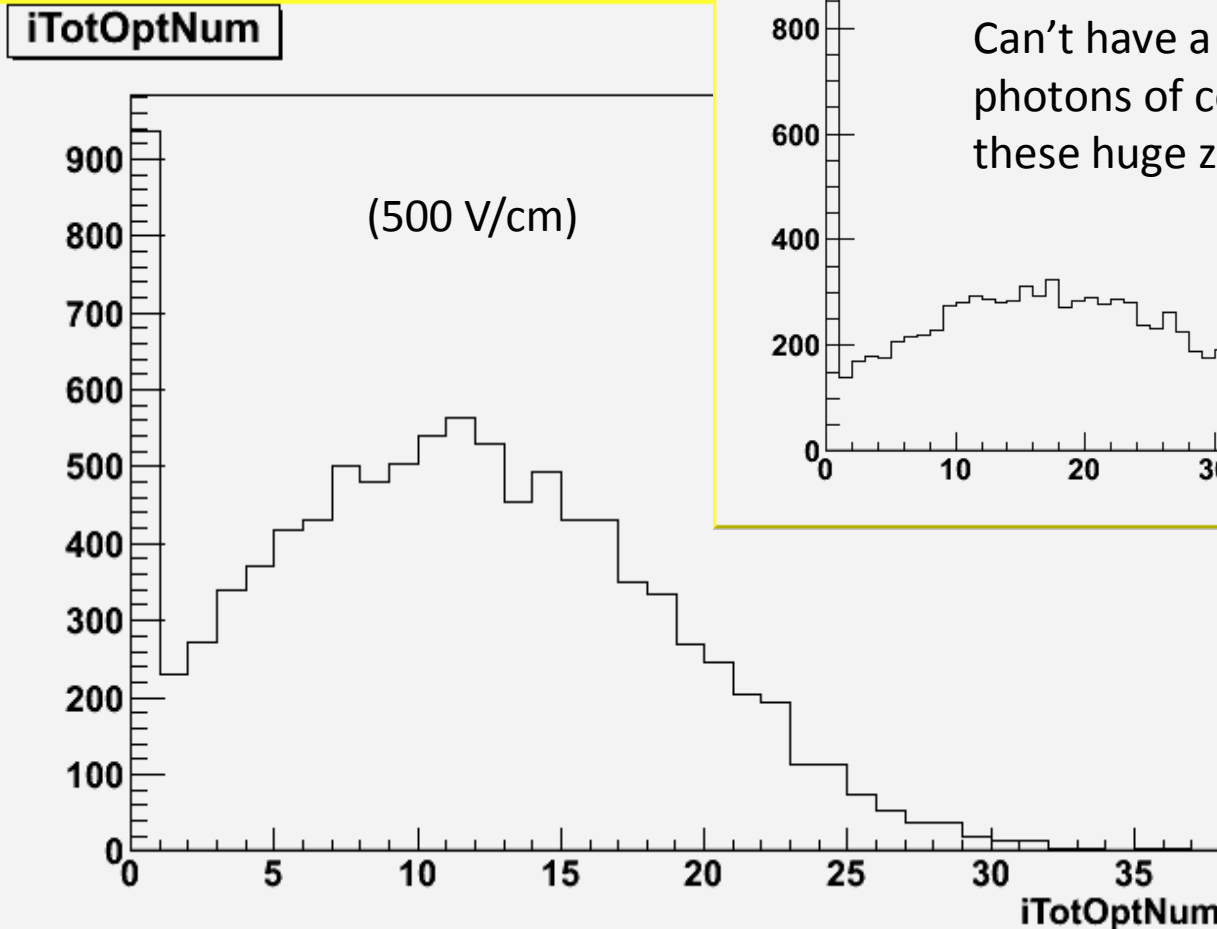- Uses ER low-E recombination probability and theoretical N_{ex}/N_i

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)

iTotOptNum

htemp	
Entries	10000
Mean	17.33
RMS	12.05

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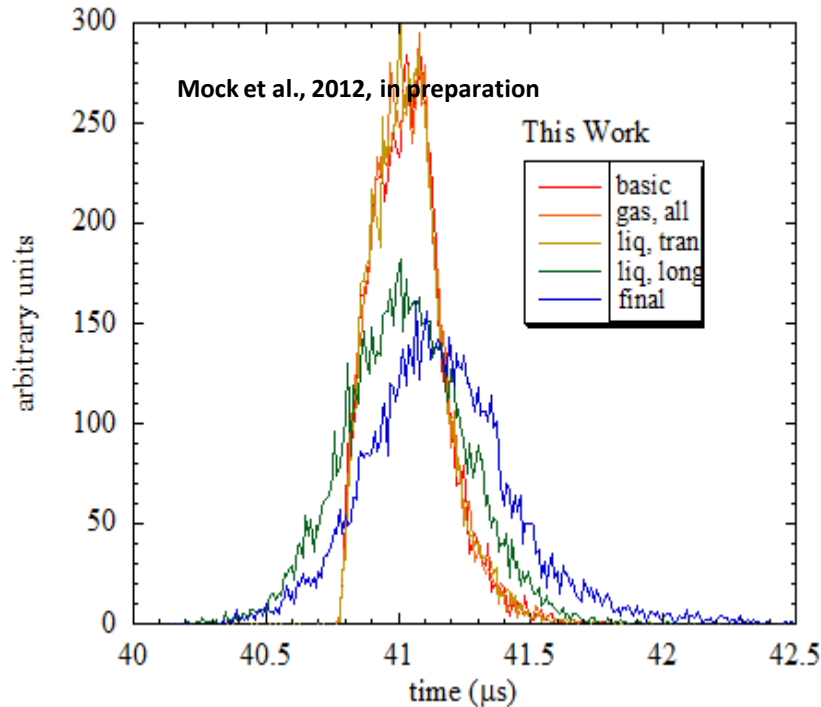
iTotOptNum

(500 V/cm)

These examples stem from the super-Poissonian fluctuations and don't include other effects, such as "Gamma-X" events
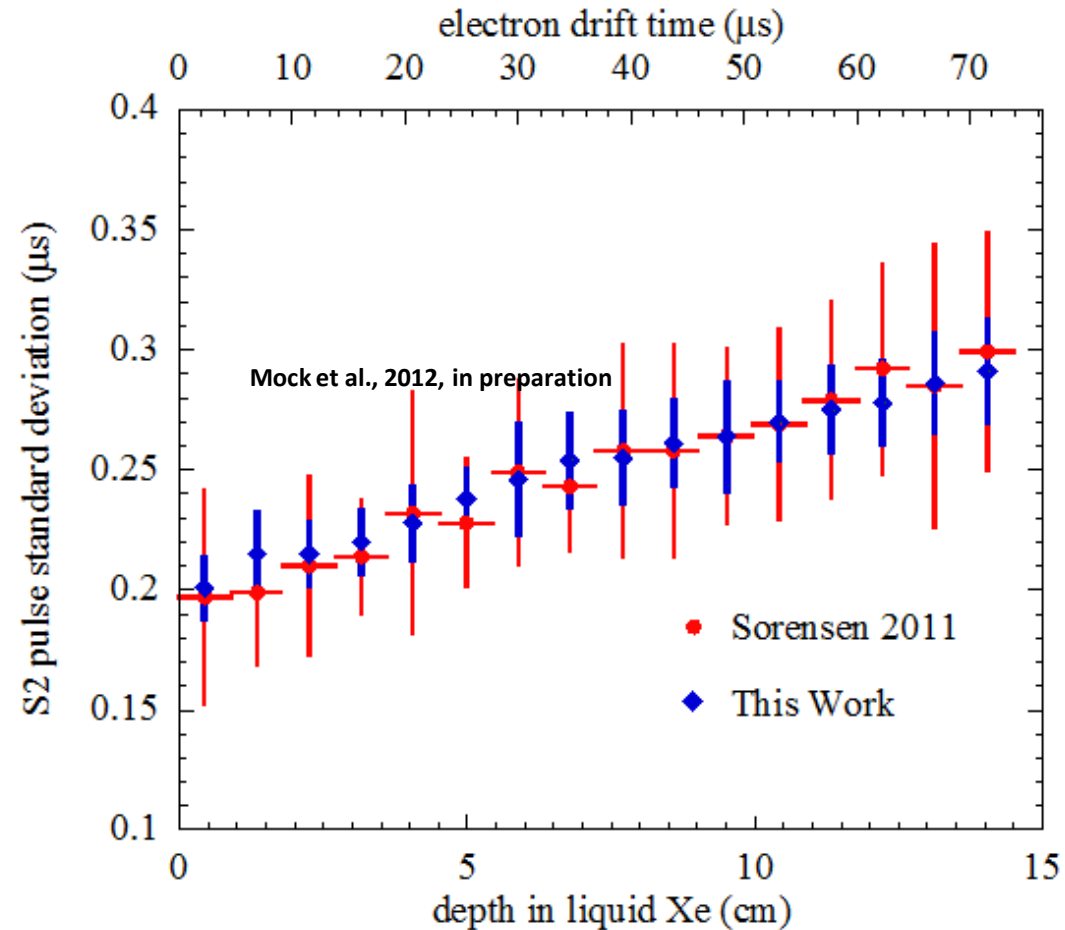
Understanding Pulse Shapes (S1)

- 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)

S1 1/e Decay Time

this is for a single decay time constant exponential fit, so singlet state is glossed over (but recombination time dominates ER)

Gammas
Electrons
Nuclear recoil
Alphas

http://nest.physics.ucdavis.edu

from
**Benchmark
Plots**

y-axis: exp τ (ns)
x-axis: energy (keV)

Understanding Pulse Shapes (S2)

Mock et al., 2012, in preparation

This Work

basic	
gas, all	
liq, tran	
liq, long	
final	

Mock et al., 2012, in preparation

● Sorensen 2011

◆ This Work

- List of included effects

  - **New G4Particle for drift e-'s**

  - Drift speed (liquid, gas)

  - Triplet, singlet lifetimes

  - Diffusion constants (transverse and longitudinal)
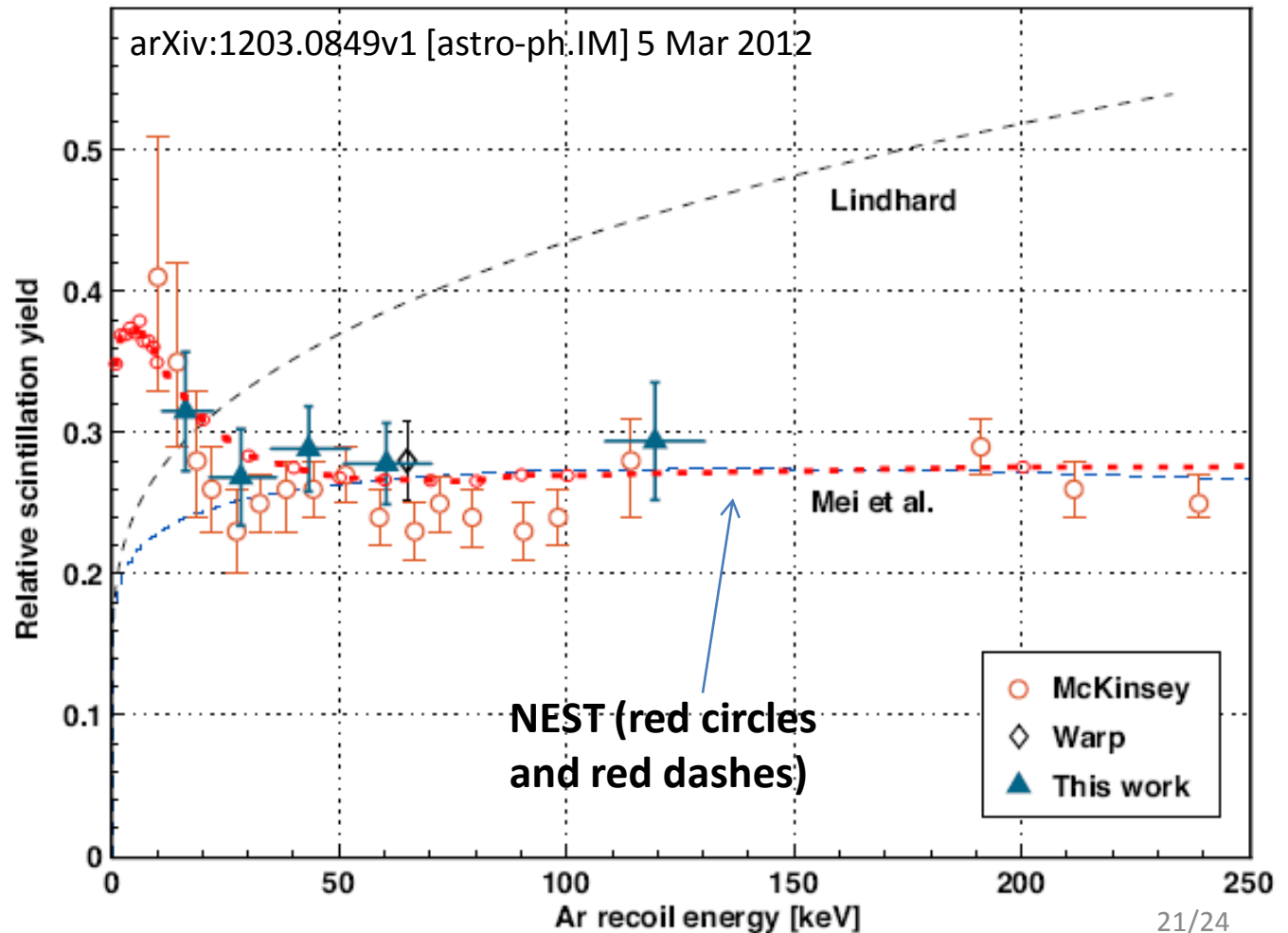
  - Electron trapping time

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

Generalizing This Work to Argon

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
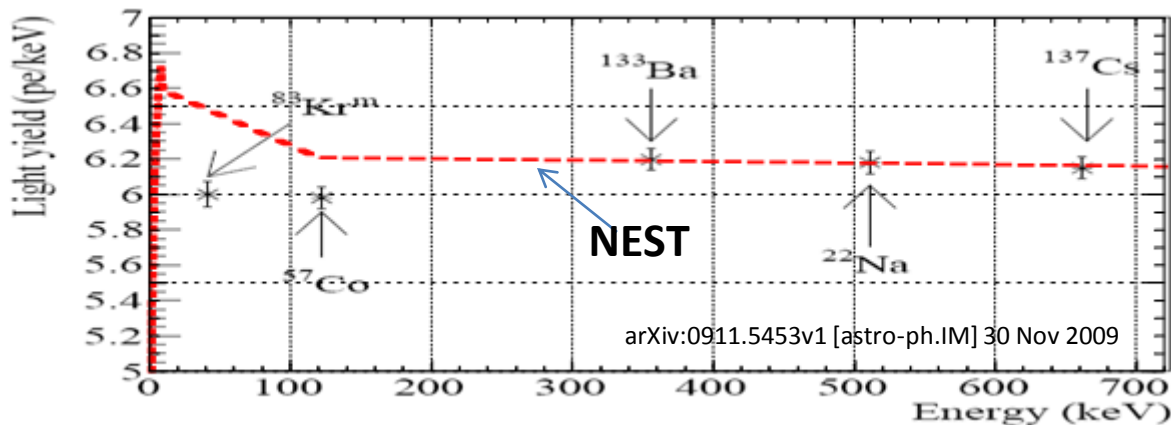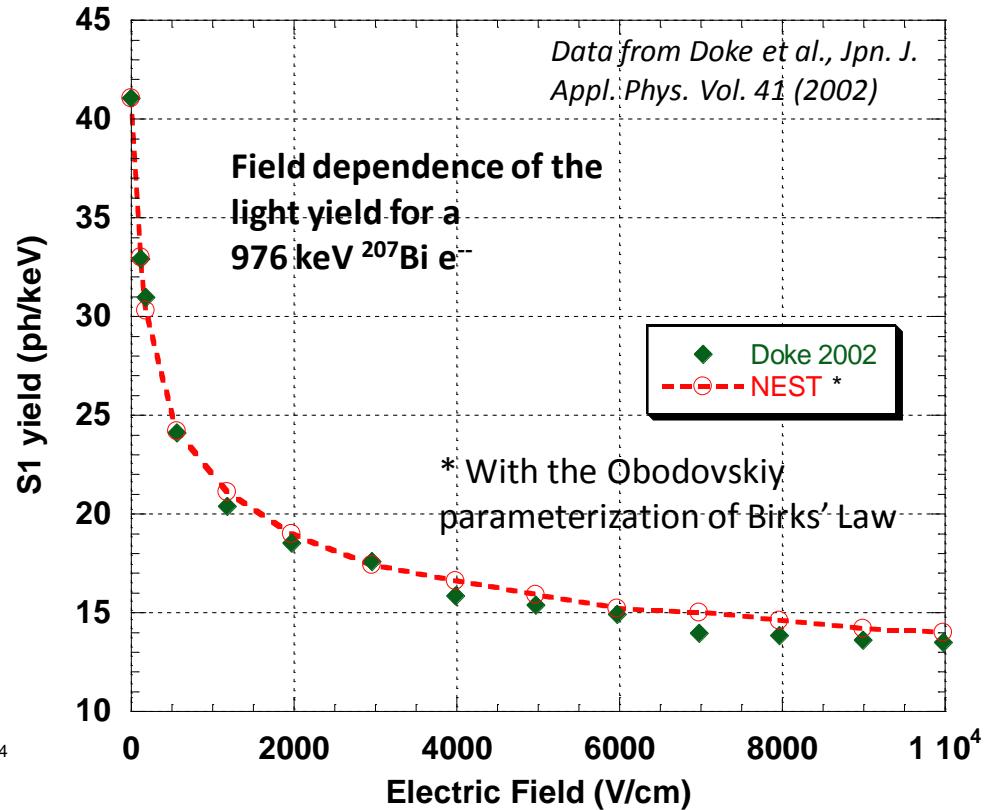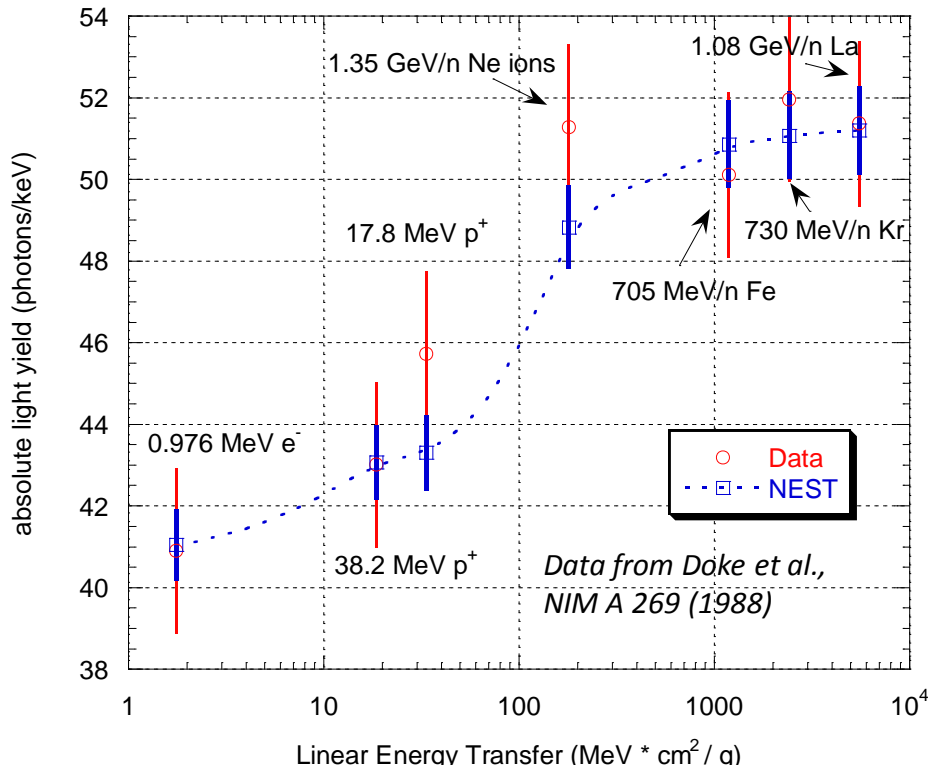
- Relative yield higher than in xenon, because the lighter argon nucleus is more efficient at transferring energy into ionization or excitation

- 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)

arXiv:1203.0849v1 [astro-ph.IM] 5 Mar 2012

Lindhard

Mei et al.

NEST (red circles and red dashes)

- ○ McKinsey
- ◇ Warp
- ▲ This work

Relative scintillation yield

Ar recoil energy [keV]

Generalizing This Work to Argon

Scintillation Yield vs. LET at Zero Field in LAr

absolute light yield (photons/keV)

1.35 GeV/n Ne ions

1.08 GeV/n La

17.8 MeV p$^+$

730 MeV/n Kr

705 MeV/n Fe

0.976 MeV e$^-$

38.2 MeV p$^+$

Data:
- Data
- NEST

Data from Doke et al., NIM A 269 (1988)

Linear Energy Transfer (MeV * cm^2 / g)

Data from Doke et al., Jpn. J. Appl. Phys. Vol. 41 (2002)

Field dependence of the light yield for a 976 keV ^{207}Bi e$^-$

S1 yield (ph/keV)

- Doke 2002
- NEST *

* With the Obodovskiy parameterization of Birks' Law

Electric Field (V/cm)

Light yield (pe/keV)

^{83}Kr^m

^{133}Ba

^{137}Cs

^{57}Co

^{22}Na

NEST

arXiv:0911.5453v1 [astro-ph.IM] 30 Nov 2009

Energy (keV)

- 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

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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....)