A Framework for Xenon Scintillation in Monte Carlo Simulations

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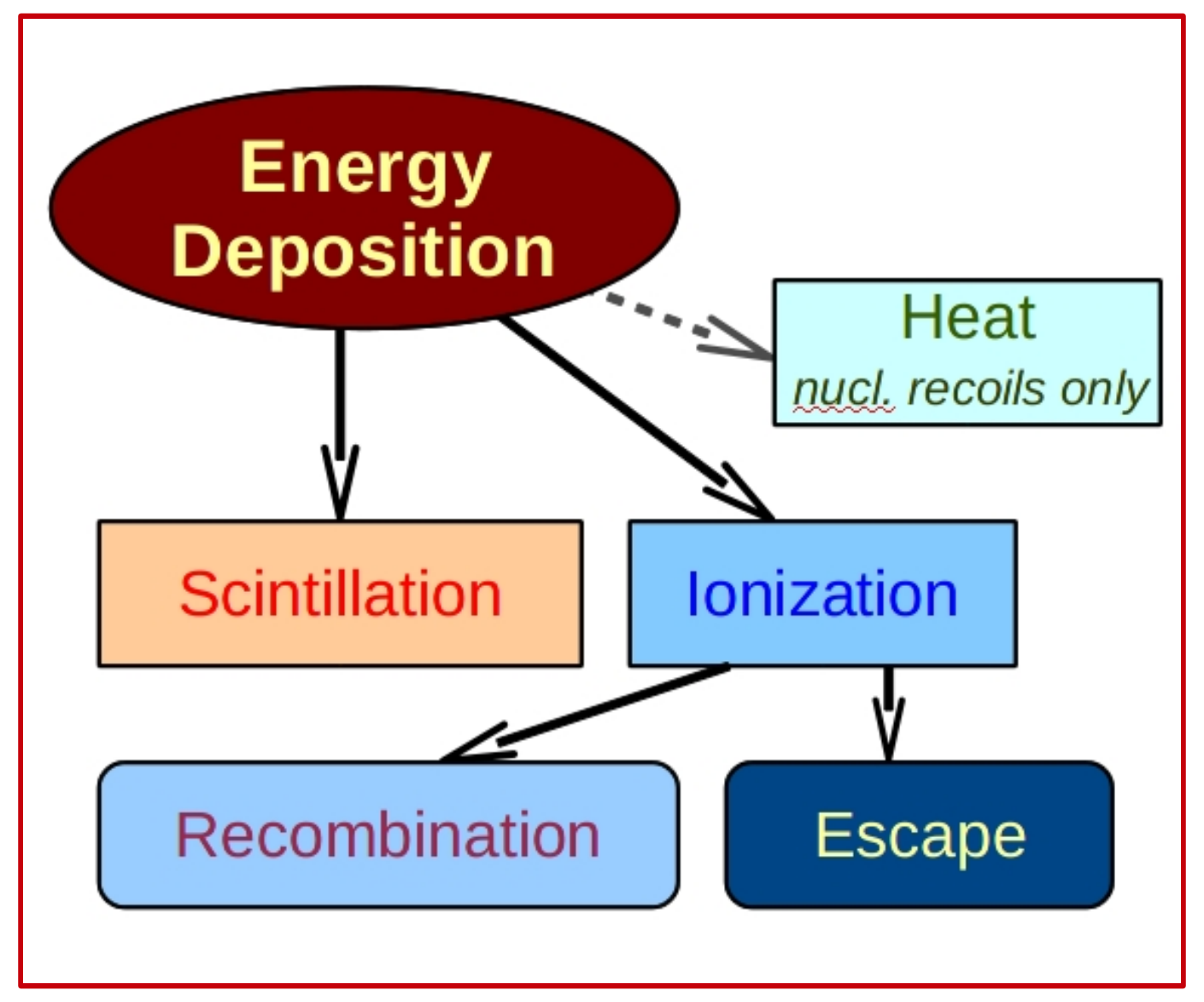
Motivation

We present a general framework for predicting xenon scintillation yield with a Monte Carlo simulation using a simple recombination model with few free parameters. We reproduce the light output from different particles over a wide range of energies and electric field magnitudes. This work is motivated by understanding liquid and two-phase xenon detectors, which are used as dark matter, double-beta decay, and general radiation detectors. The simplicity of our model suggests that it can be extended to any noble element.

Excitation and Ionization Model



An interaction in xenon generates excitons and electron-ion pairs. Ionized electrons can recombine to form more excitons, or escape in the presence of an electric field. Nuclear recoils may lose energy to "heat" by leading to additional nuclear recoils. Excitons lead to scintillation and escaping electrons can lead to a charge signal.

The work function (W) is the energy required for excitation or ionization. If N_{ex} and N_i are the excitons and ions produced by an interaction depositing energy E_{dep} and r is the recombination probability, then the following equations govern the number of photons (N_{ph}) and electrons (N_e) produced, the detectable quanta:

$$E_{dep} = W(N_{ex} + N_i)$$
$$N_{ph} = N_{ex} + rN_i$$
$$N_e = N_i(1-r)$$

We consider two models to describe the recombination probability, the Jaffe columnar model and the Thomas-Imel box model [1,2,3]. The Jaffe model is well-suited for long particle tracks, and is dE/dx-dependent:

$$r = \frac{A\frac{dE}{dx}}{1+B\frac{dE}{dx}} + C, \quad C = 1 - A/B$$

For short tracks, those shorter than the electron-ion thermalization distance, the recombination probability is calculated using the Thomas-Imel model, which is independent of dE/dx:

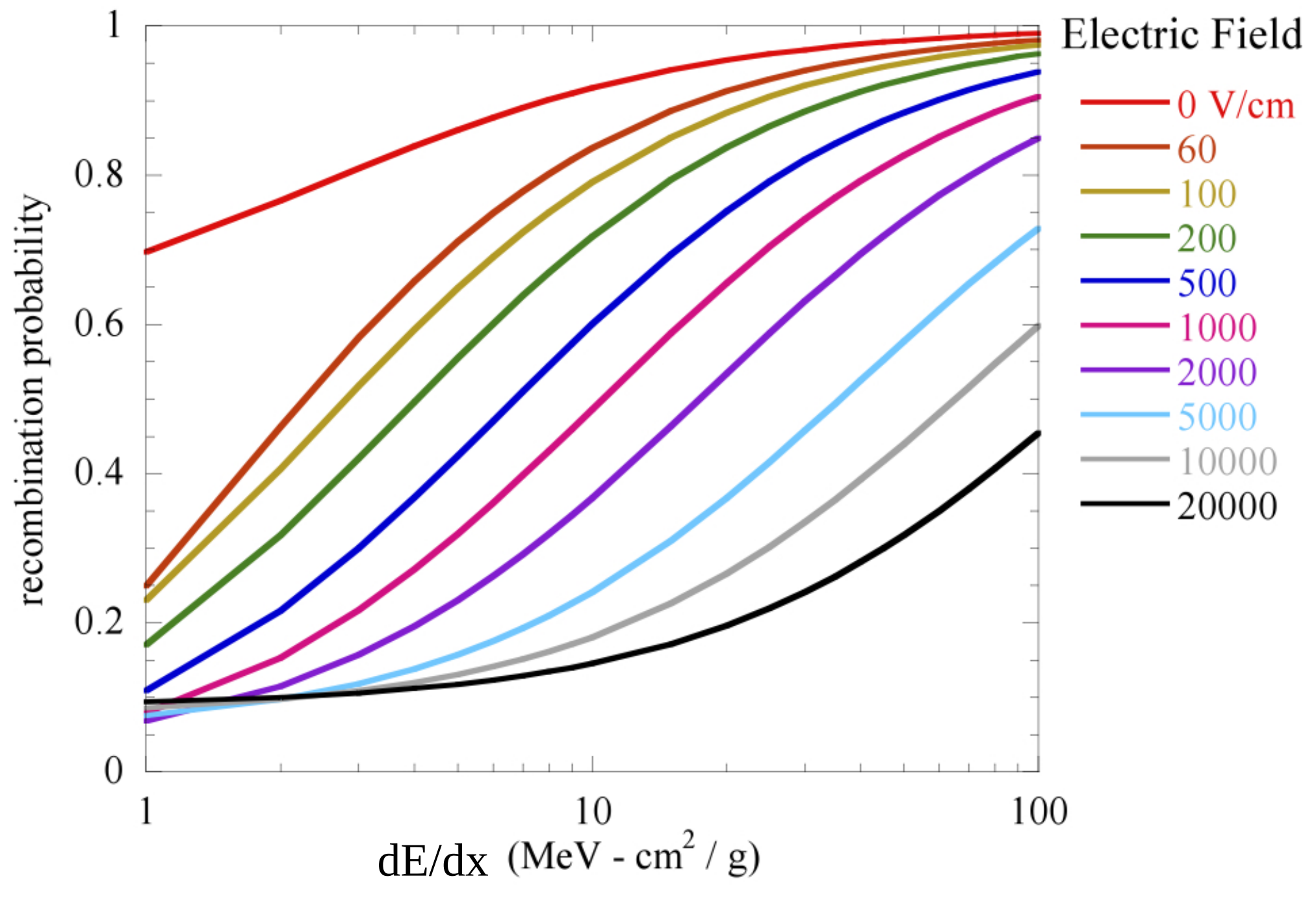
$$r = 1 - \frac{\ln(1+\xi)}{\xi}, \quad \xi = \frac{N_i\alpha}{4a^2v}$$

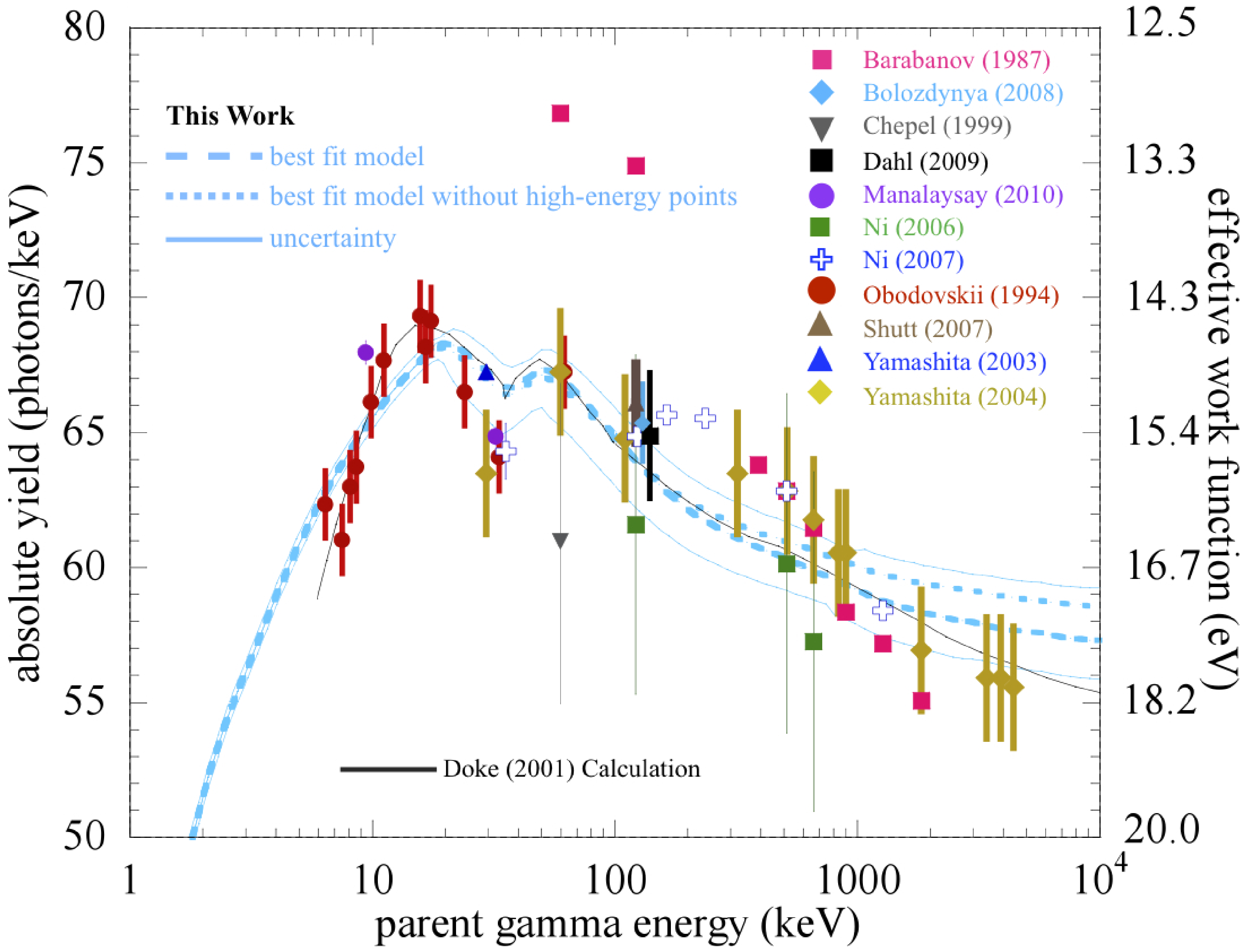
Where α is a constant related to electron and hole mobilities, a is the effective "box" size defining the ionization density, and v is the mean ionized electron speed.

Zero-Field Scintillation Yield From Electron Recoils

By treating A, B, and $\alpha/(a^2v)$ from the models as free parameters, we match compiled data for zero-field gamma ray scintillation. The best fit successfully reproduces different empirically observed features in the spectrum. Our best fit uses W=13.7 eV, A=0.18, B=0.42, $\alpha/(a^2v)$=0.19, and a ratio of excitons to ions of 0.06.

Example semi-empirical recombination probability curves as a function of electric field and dE/dx. The red line for zero field is used to produce the plot below. The other recombination probabilities shown here are used to produce the electric field plots at right. These probabilities are not deterministic: our simulations include stochastic variation in the recombination.

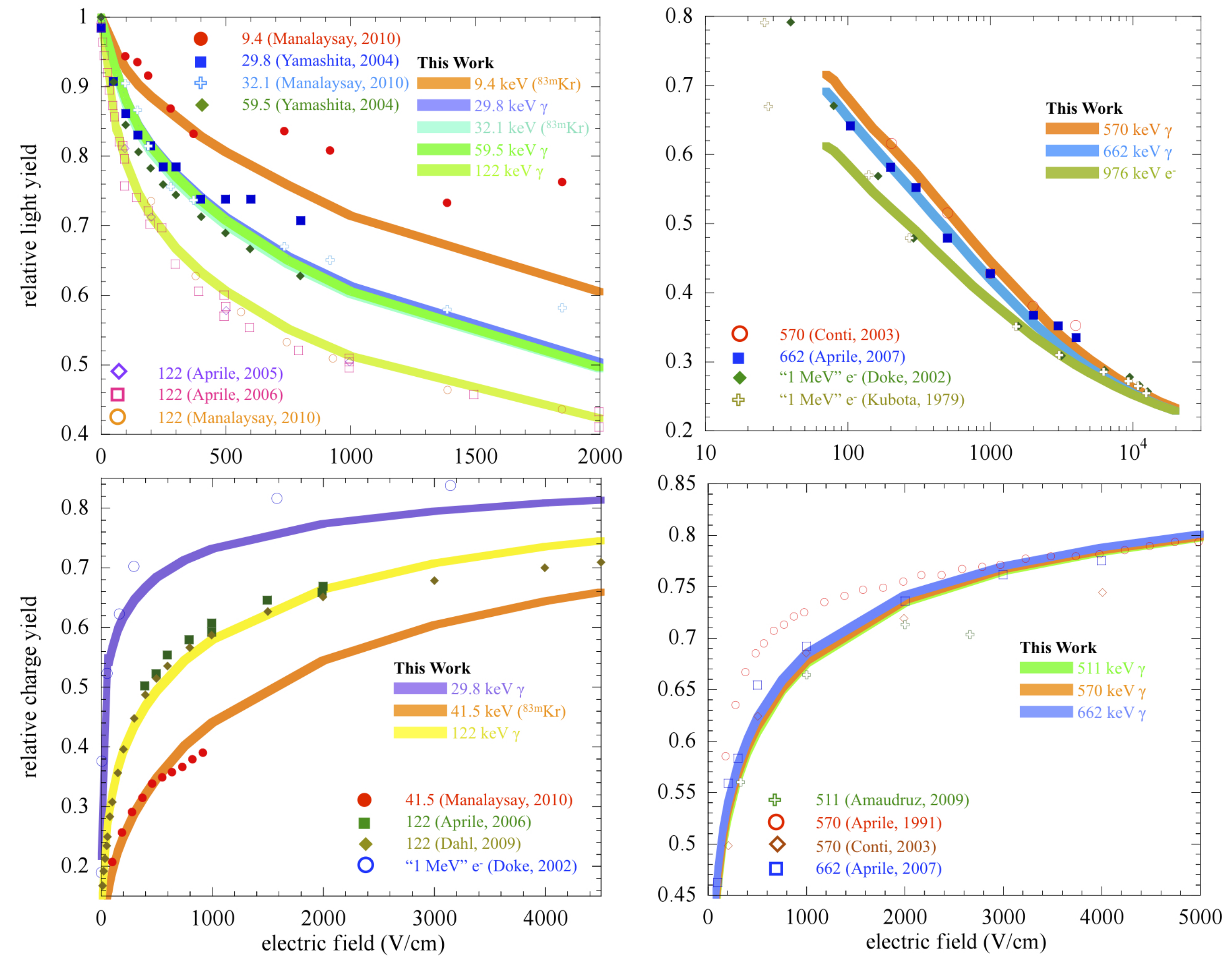




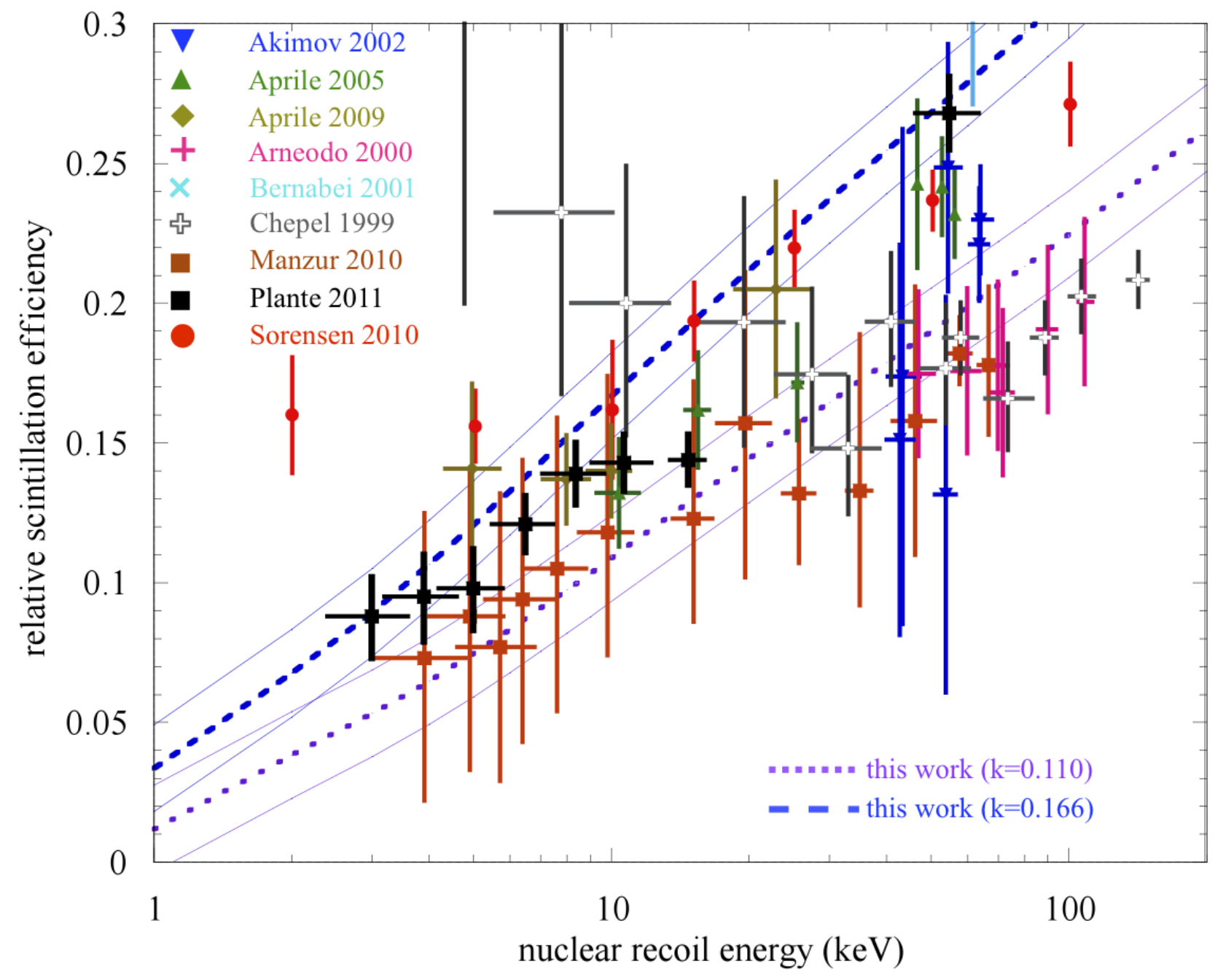
The light blue curve shows the absolute light yield extracted from a Monte Carlo simulation in GEANT4 that tracks individual energy depositions for different parent gamma ray energies. A dashed line indicates the best fit to the data, while solid lines denote the 1σ error band. Our model successfully shows a low energy decrease in yield, a dip due to enhancement in low-energy electron production at ~35 keV, and a decrease of scintillation at higher energy. Empirical data quoted as relative yield is converted to absolute yield in order to be effectively utilized. This is done by using gamma rays for which absolute yield measurements are available, such as 122 keV, as conversion keys for the relative data at higher and lower energies. Note that the lower-energy end at left is not an extrapolation but actual Monte Carlo prediction.

Scintillation and Ionization Yields With Electric Field

As electric field increases the recombination probability falls. We adjust our three free parameters in order to fit all available data for electron recoils at different field strengths. Predictably, the charge yield (bottom half) is anti-correlated to the light yield (top) because the total available energy is fixed.



Predicting Nuclear Recoil Scintillation Yield



Using the same parameters from electron recoil, adding only the Lindhard factor, we can successfully reproduce nuclear recoil light yields. We show two possible scenarios: pure Lindhard theory (top band) and Lindhard theory as modified by Hitachi (lower band) [4,5]. Scintillation yields are reported relative to the 122 keV gamma.

Conclusions

We have demonstrated an effective approach to simulating xenon scintillation and ionization. Our work is consistent with the vast majority of experimental data. However, instead of directly fitting data on yields we approach the problem at the level of simulating the probability for individual ionized electrons to recombine. Our model has the advantage of few free parameters, making it simple to implement in the Monte Carlo simulation of any xenon experiment.

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