Ionization efficiency at sub-keV energies for crystals and noble liquids

Y. Sarkis
Presented by Daniel Baxter

Instituto de Ciencias Nucleares, UNAM Mexico

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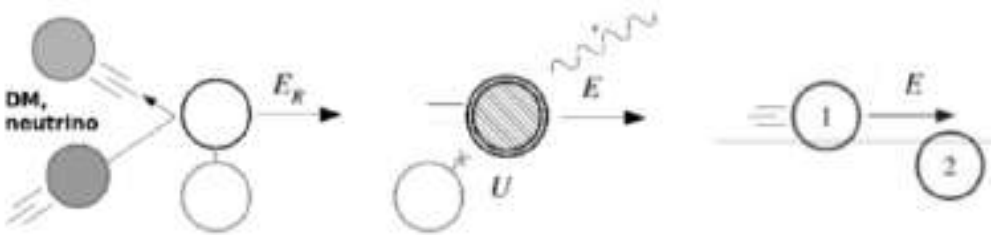
Contents

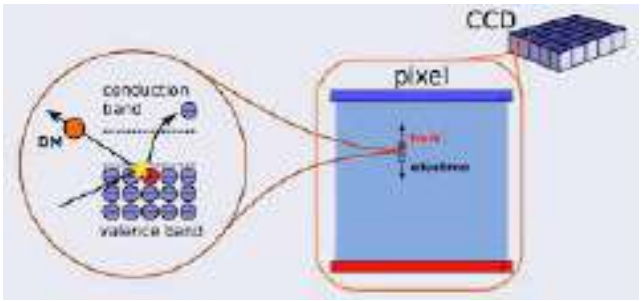
Useful links:

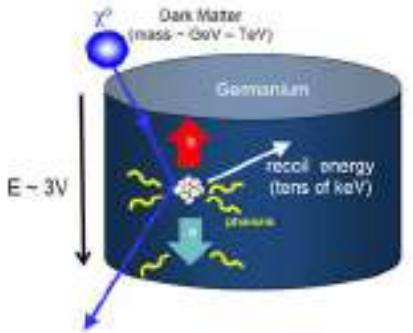
(A) Magnificent CEνNS(2021)
(A) Magnificent CEνNS(2020)
(B) XXXV DPC-SMF meeting (2021)

Introduction (Ionization only detectors)

Deposited energy splits in;
E_ν : Nuclear collisions. ($\bar{\nu}$[1])
E_I : Ionization (visible) energy [$\mathrm{keV_{ee}}$] ($\bar{\eta}$).







- $quenching = \frac{\text{total ionization energy}}{\text{total deposited energy}} = f_n = \frac{\bar{\eta}}{\varepsilon_R}$.
- $\varepsilon_R = \bar{\eta} + \bar{\nu}$, where ε_R is the recoil energy.
- Energy u is lost to some disruption of the atomic bonding: $\varepsilon_R = \varepsilon + u$.
- The ion moves with a kinetic energy ε.
- This sets a cascade of slowing-down processes that dissipate the energy E throughout the medium.

[1] Using dimensionless units ($\varepsilon = 16.26E(\mathrm{keV})/\mathrm{Z_1Z_2}(\mathrm{Z_1^{0.23}} + \mathrm{Z_2^{0.23}})$)

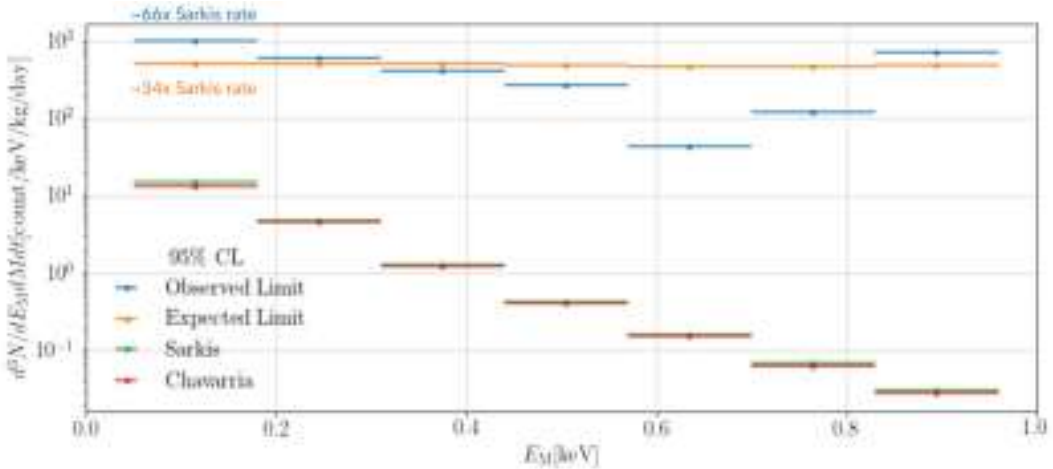
Signals affected by quenching

- For DM or CEνNS searches with pure crystals the quenching plays an important role for calibration and efficiency.
- Different quenching, change significantly the rate for CEνNs signal.

$$\frac{dR}{dE_I} = \frac{dR}{dE_R} \underbrace{\frac{1}{f_n}\left(1 - \frac{E_I}{f_n}\frac{df_n}{dE_I}\right)}_{\frac{dE_R}{dE_I}}$$

$$f_n = \frac{E_I}{E_R},$$

The visible energy spectrum is shifted to lower energies, due to the QF.



CEνNS limits for different quenching [JHEP 05 (2022), 017].

f_n **depends mainly on electronic stopping** S_e**.**
If $S_e = 0$ then $f_n = 0$.

Basic integral equation and approximations

(T_n : Nuclear kinetic energy and T_{ei} electron kinetic energy.)
Energy conservation for atomic motion $\bar{\nu}$ in all successive collisions,

$$\underbrace{\int d\sigma_{n,e}}_{\text{total cross section}} \left[\underbrace{\bar{\nu}\left(E - T_n - \sum_i T_{ei}\right)}_{\text{All scatter-ions ions}} + \underbrace{\bar{\nu}\left(T_n - U\right)}_{\text{All Target ions}} + \underbrace{\bar{\nu}(E)}_{\text{Total initial energy}} + \underbrace{\sum_i \bar{\nu}_e\left(T_{ei} - U_{ei}\right)}_{\text{Electrons contribution}} \right] = 0 \quad (1)$$

Lindhard's (five) approximations

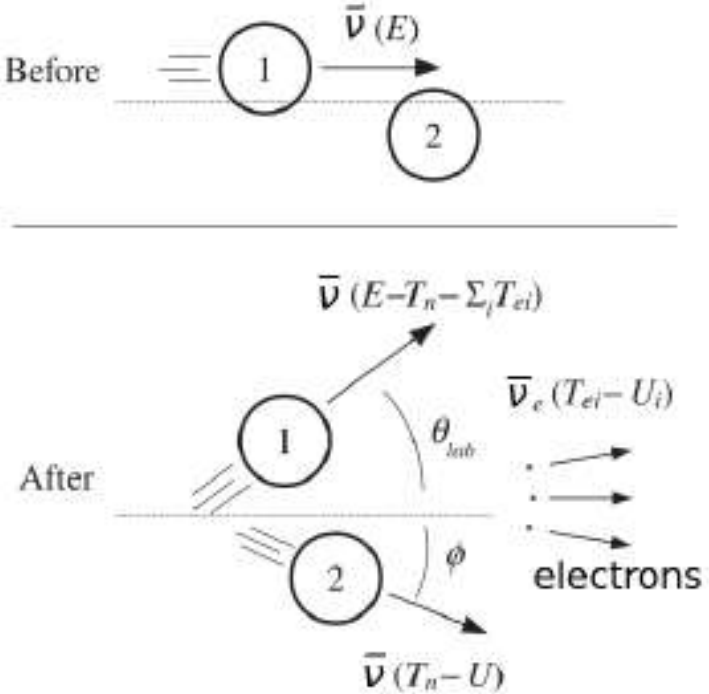
I. Neglect contribution to atomic motion coming from electrons.

II. **Neglect the binding energy, U = 0. (Now taken into account)**

III. Energy transferred to electrons is small compared to that transferred to recoil ions.

IV. Effects of electronic and atomic collisions can be treated separately.

V. T_n is also small compared to the energy E.



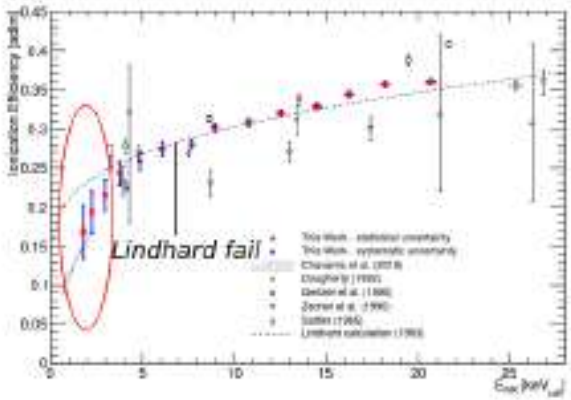
Lindhard simplified equation

Using the five approximations Lindhard deduced an integral simplify equation,

$$\underbrace{(k\varepsilon^{1/2})}_{S_e}\bar{\nu}'(\varepsilon) = \int_0^{\varepsilon^2} \underbrace{dt\frac{f\left(t^{1/2}\right)}{2t^{3/2}}}_{d\sigma_n}[\bar{\nu}(\varepsilon - t/\varepsilon) + \bar{\nu}(t/\varepsilon) - \bar{\nu}(\varepsilon)], \qquad (2)$$

but since binding energy was neglected is only valid at high energies, since $\bar{\nu}(\varepsilon \to 0) \to \varepsilon$, by the above equation we get $\bar{\nu}'(0) = 0$!.

- First principles (e) stopping power $S_e = k\varepsilon^{1/2}$, $k = 0.133Z^{2/3}/A^{1/2}$.
- Lindhard deduce a parametrization valid at high energies (U=0).
- But fails below 4 keV.



PRD Chavarria et all, 94, 082007(2016)

$$\bar{\nu}_L(\varepsilon) = \frac{\varepsilon}{1 + kg(\varepsilon)},\ g(\varepsilon) = 3\varepsilon^{0.15} + 0.7\varepsilon^{0.6} + \varepsilon.$$

Simplified equation with binding energy

Binding energy effects may be relevant at low energies. We include this by,

- Relaxing approximations II, III and V.
- Considering U constant, Lindhard $S_e = k\varepsilon^{1/2}$ (this is the simplest case).
- Nuclear stopping $d\sigma_n(t)$ with $t = \varepsilon^2 \sin^2(\theta/2)$.
- We solve for $\bar{\nu}$ then $\bar{\eta} = \varepsilon_R - \bar{\nu}$ and, $f_n = \bar{\eta}/\varepsilon_R$.

(Y. Sarkis et al, Phys. Rev. D 101, 102001 (2020))

$$-\frac{1}{2}k\varepsilon^{3/2}\bar{\nu}''(\varepsilon) + \underbrace{k\varepsilon^{1/2}}_{S_e\ :\ Lindhard}\ \bar{\nu}'(\varepsilon) = \int_{\varepsilon u}^{\varepsilon^2} \underbrace{dt\frac{f\left(t^{1/2}\right)}{2t^{3/2}}}_{d\sigma_n}[\bar{\nu}(\varepsilon - t/\varepsilon) + \bar{\nu}(t/\varepsilon - u) - \bar{\nu}(\varepsilon)] \tag{3}$$

- Threshold at $\varepsilon_R^{threshold} = 2u$.
- Inter-atomic potential dependent $f(t)$.
- e.g T.F., Moliere, AVG and Ziegler

First results for Si

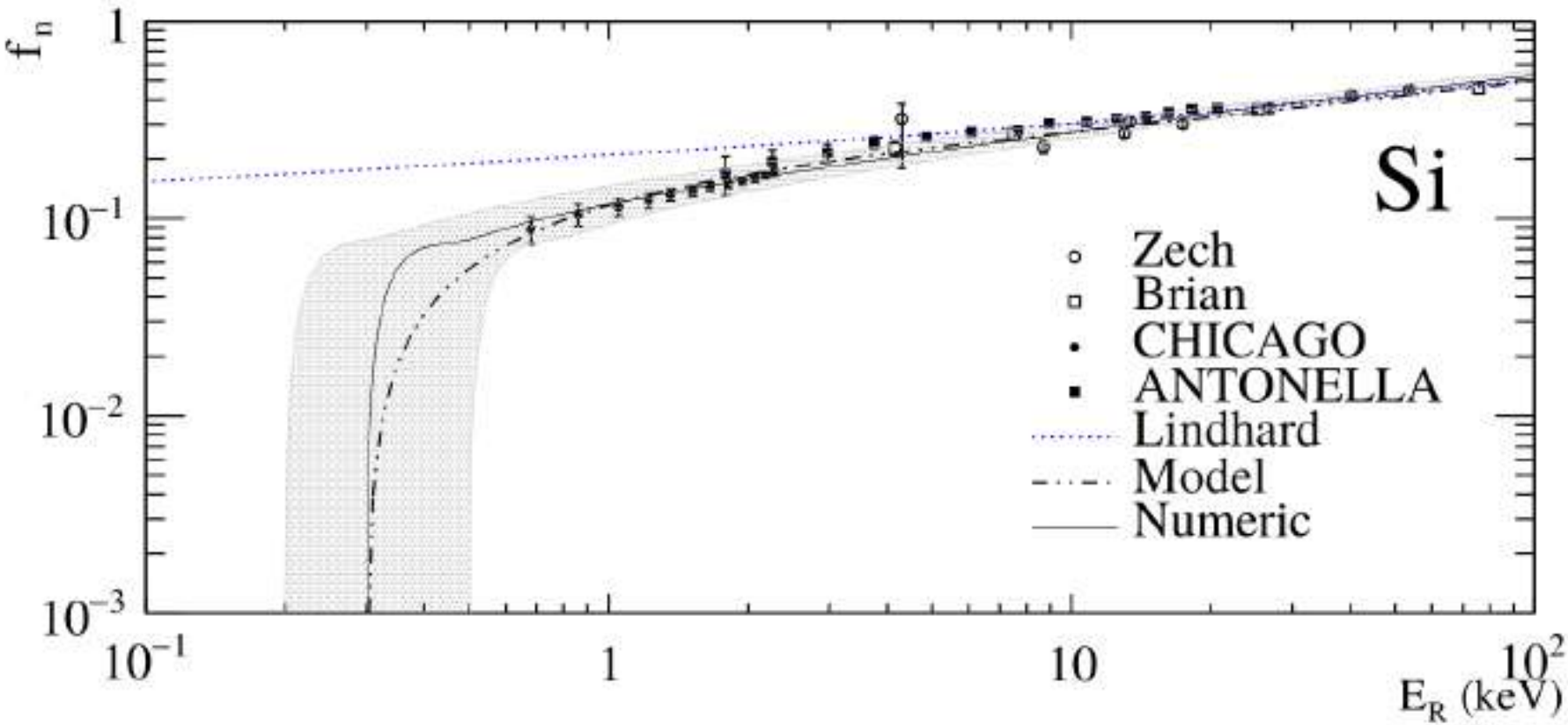


Figure: QF measurements for Si, compared with Lindhard model, the ansatz and the numerical solution; U = 0,15 keV y k = 0,161.

Improvements of the model

- **For Si, constant U, gives a cut off too high compared to the expected threshold given by the energy to create a Frenkel-pair (≈ 30 eV).**
- A varying binding energy model is proposed;
  - Low energies just considered the Frenkel energy.
  - High energy consider electron inner excitations, using T.F theory.
- **Lindhard electronic stopping is not valid at low energies.**
- It doesn't considered Coulomb repulsion effects and electron stripping.
- We can also add electronic straggling $\Omega^2 = \langle \delta E - \langle \delta E \rangle \rangle^2$ ($\frac{d\Omega^2}{d\rho} \equiv W$) effects to the model.

$$-\frac{1}{2}\varepsilon S_e(\varepsilon)\left(1+\frac{W(\varepsilon)}{S_e(\varepsilon)\varepsilon}\right)\bar{\nu}''(\varepsilon)+S_e(\varepsilon)\bar{\nu}'(\varepsilon)= \int_{\varepsilon u}^{\varepsilon^2} dt \frac{f\left(t^{1/2}\right)}{2t^{3/2}}[\bar{\nu}(\varepsilon - t/\varepsilon)+\bar{\nu}(t/\varepsilon - u)-\bar{\nu}(\varepsilon)], \tag{4}$$

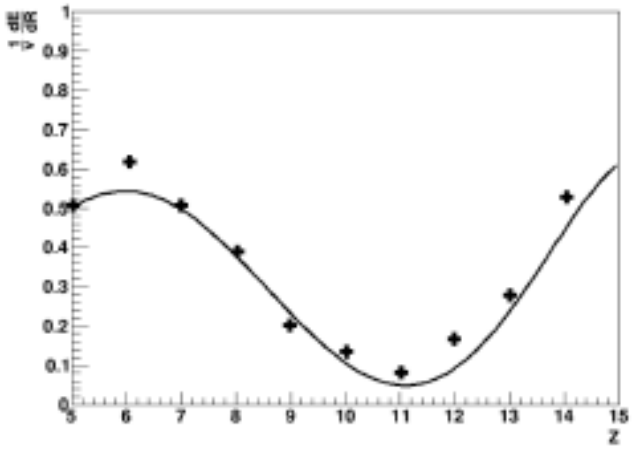
High energy effects (> 10 keV) for $S_e(\varepsilon)$

§ Bohr Stripping

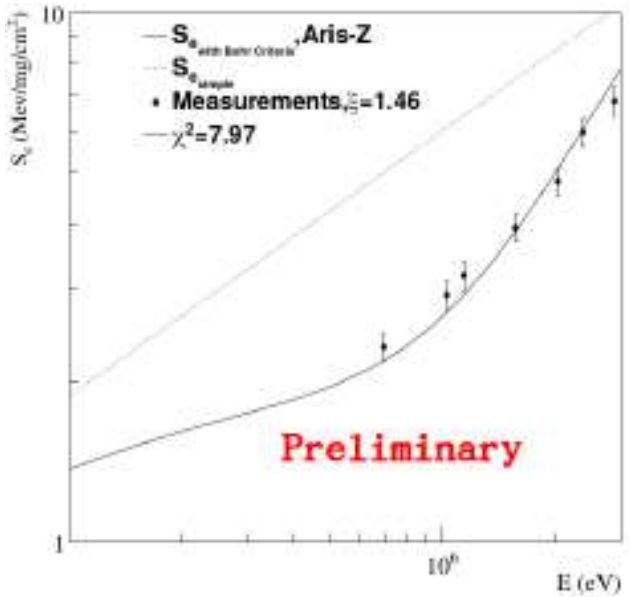
- Electrons can be lost according to momentum transferred.
- The effective number of electrons obeys $Z^{\dagger} \approx Ze^{-v/Z^{2/3}v_0}$.
- $S_e \propto Z^{\dagger}$, this leads to damping.

§ Z Oscillations

- When the ion charge changes, the transport cross section σ_T changes.
- Phase shift is appear to maintain neutrality of electron Fermi gas.
- S_e may be affected by this effect at energies $v \ll v_0 Z^{2/3}$.Since $S_e \propto \sigma_T$.



▫ Z oscillation for Si.



▫ S_e vs data

Low energy effects for S_e

§ *Coulomb repulsion effects*

- At low energies S_e departures from velocity proportionality.
- Colliding nuclei will partially penetrate the electron clouds.

$$S_e = (\Xi) N m v \int_0^\infty v_F \sigma_{tr}(v_F) N_e dV \rightarrow (\Xi) N m v \int_R^\infty v_F \sigma_{tr}(v_F) N_e dV$$

R distance closest approach and Ξ is a geometrical factor[4] , negligible for $Z < 20$.

- Three models will be considered; **Tilinin[2], Kishinevsky[3] and Arista[4]**
- Models change details of the inter-atomic potential.
- Hence affect $f(t^{1/2})$ and S_e at low energies.

[2] I.S.Tilinin Phys. Rev. A 51, 3058 (1995)

[3] Kishinevsky, L.M., 1962, Izv. Akad. Nauk SSSR, Ser. Fiz. 26, 1410.

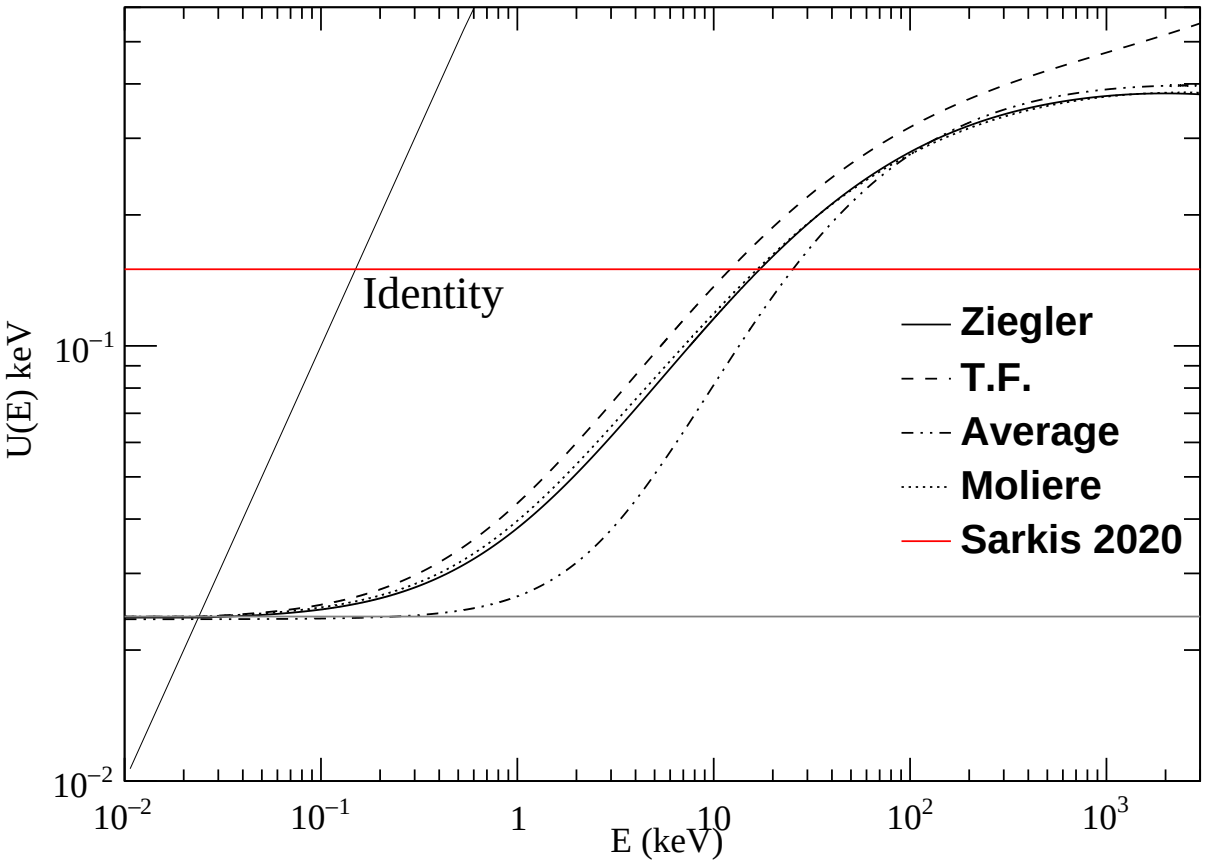
[4] J.M. Fernández-Varea, N.R. Arista, Rad. Phy. and C.,V 96, 88-91, (2014),

Binding energy model

The model consider:

- Frenkel pair creation energy, U_{FP}.
- Atomic binding with DFT theory, $U_{TF}(E)$.
- $U(E) = U_{FP} + U_{TF}(E)$

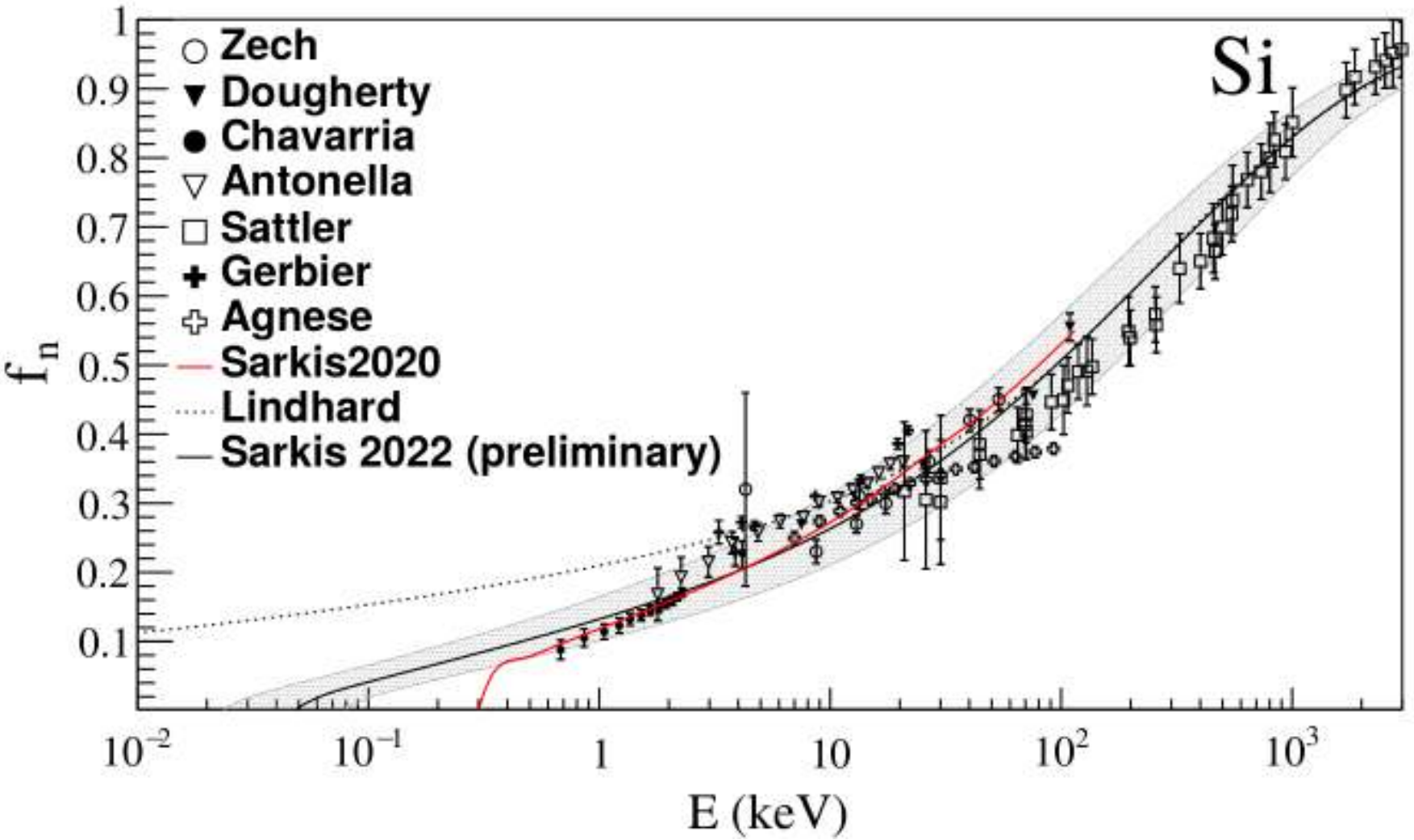
$$U_{FP} = 23.54^{+9.63}_{-12.04} \text{ eV}$$



The DFT depends on the screening function used in the inter-atomic potential.

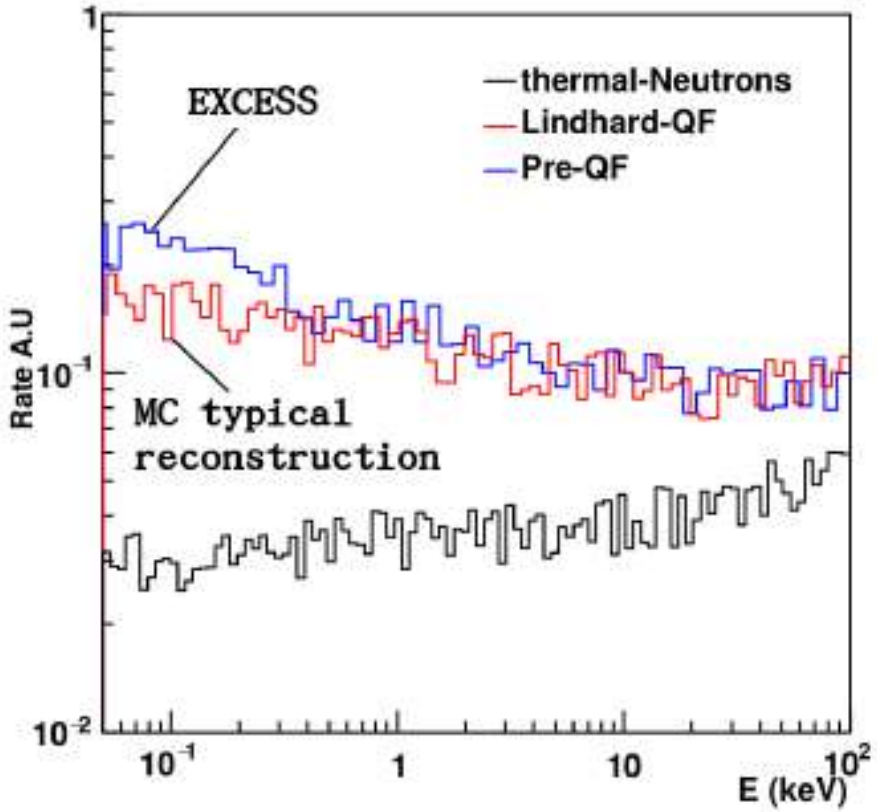
QF Results (Si) up to 3 MeV.

We fit the inter-atomic scale parameter, that scales S_e, S_n and has important effects at low energies.



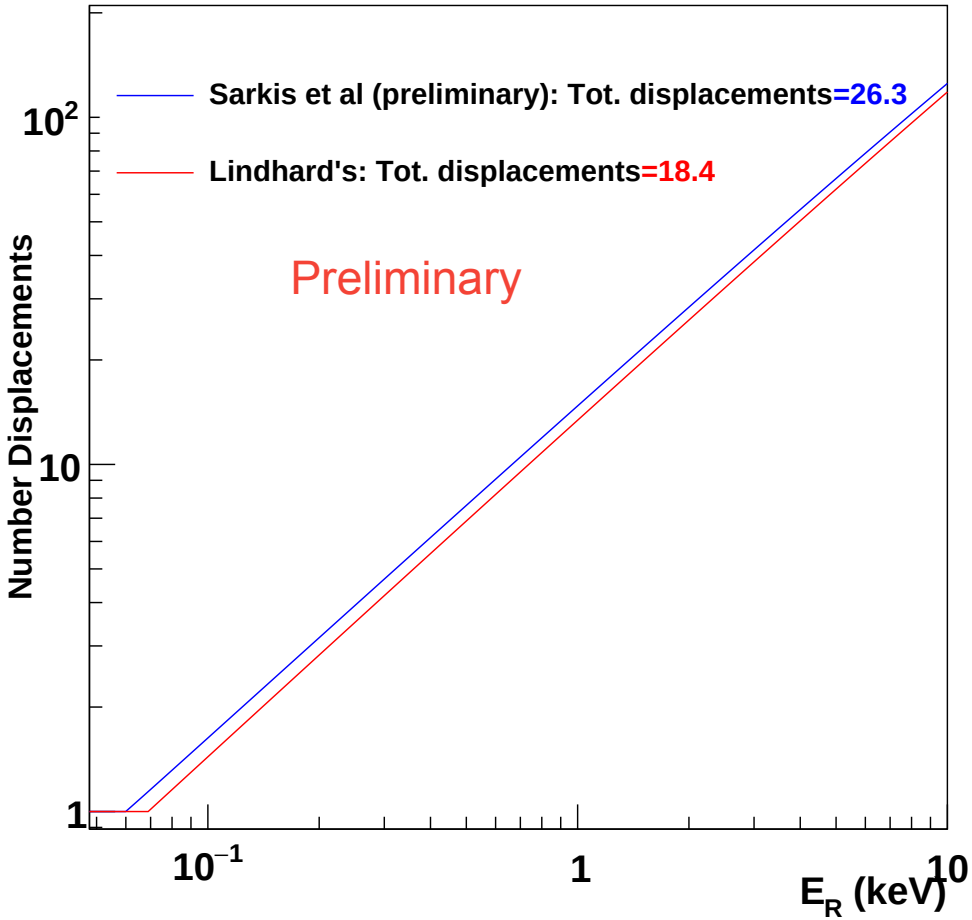
EXCESS for flat low energy signals

- We can expect an EXCESS from a flat spectrum signal,.e.g. thermal Neutrons.
- By comparing spectrum reconstruction from Lindhard QF and our new QF model.
- Lindhard QF is usually used by MC simulations, etc.



Energy loss by defect creation in Si

- Frenkel pairs (Fr-P) can create peak signals near threshold.
- We can compute the number of Fr-P by using Kinchin and Pease model combined with our solution for $\bar{\nu}$; $N_{Fr-P} = 0.8\bar{\nu}/2u_{Fr}$.



Results (Ge) with Collar recent data

For Ge study we have to consider a geometrical factor, mentioned by Tilinin and only significant for high Z ($Z > 20$).

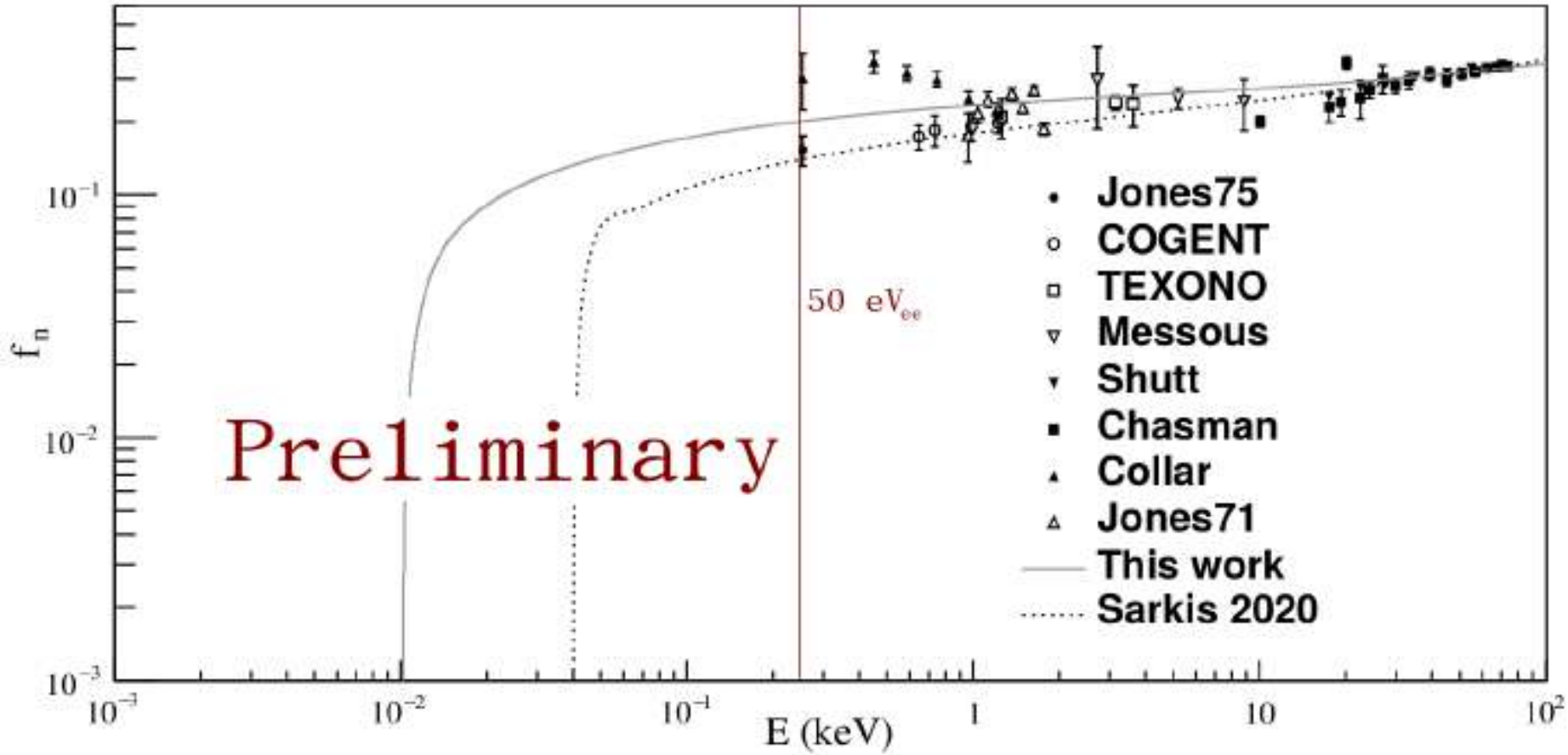


Figure: Germanium QF model with straggling, **geometrical factor**, low and high energy effects.

Noble gases ionization response

- Dual-phase noble liquid time projection chambers (TPCs) have yielded, a competitive sensitivity for the search for WIMPs.
- Reconstruction is done by exploiting the full anticorrelation between the S1 (scintillation photons n_γ) and S2 (ionized electrons n_e).

$$E_{\mathrm{er}} = W\left(\frac{S1}{g_1} + \frac{S2}{g_2}\right), \quad \rightarrow E_R = W\left(n_\gamma + n_e\right)/f_n,$$

- With $W_{Ar} = 19.5$ eV and $W_{Xe} = 13.7$ eV, is the average energy required to produce an excitation or ionization for Ar and Xe.
- It is usually to assume that each excited atom leads to one scintillation photon.
- And that each ionized atom leads to a single electron unless it recombines

Thomas Imel Box Model

- We have $N_i + N_{ex} = n_\gamma + n_e$ independent of recombination.
- The fraction of ionizations is predicted by the Thomas-Imel box model

$$Q_y^{\mathrm{ER}} = \frac{N_{\mathrm{i.e.}}}{E_{\mathrm{er}}} = \frac{(1-r)N_i}{E_{\mathrm{er}}}, \quad 1 - r = \frac{1}{\gamma N_i} \ln\left(1 + \gamma N_i\right)$$

- Where $N_i = f_n(\frac{E_R}{W(1+\alpha)})$, where α and γ are free parameters.
- f_n can be computed with our model.
- This model has been shown to work well for spatially small tracks.
- In the following we show the Charge and Light Yiels for Ar and Xe, using the constant binding energy model and $S_e = k\varepsilon^{1/2}$.

Xenon Charge Yield

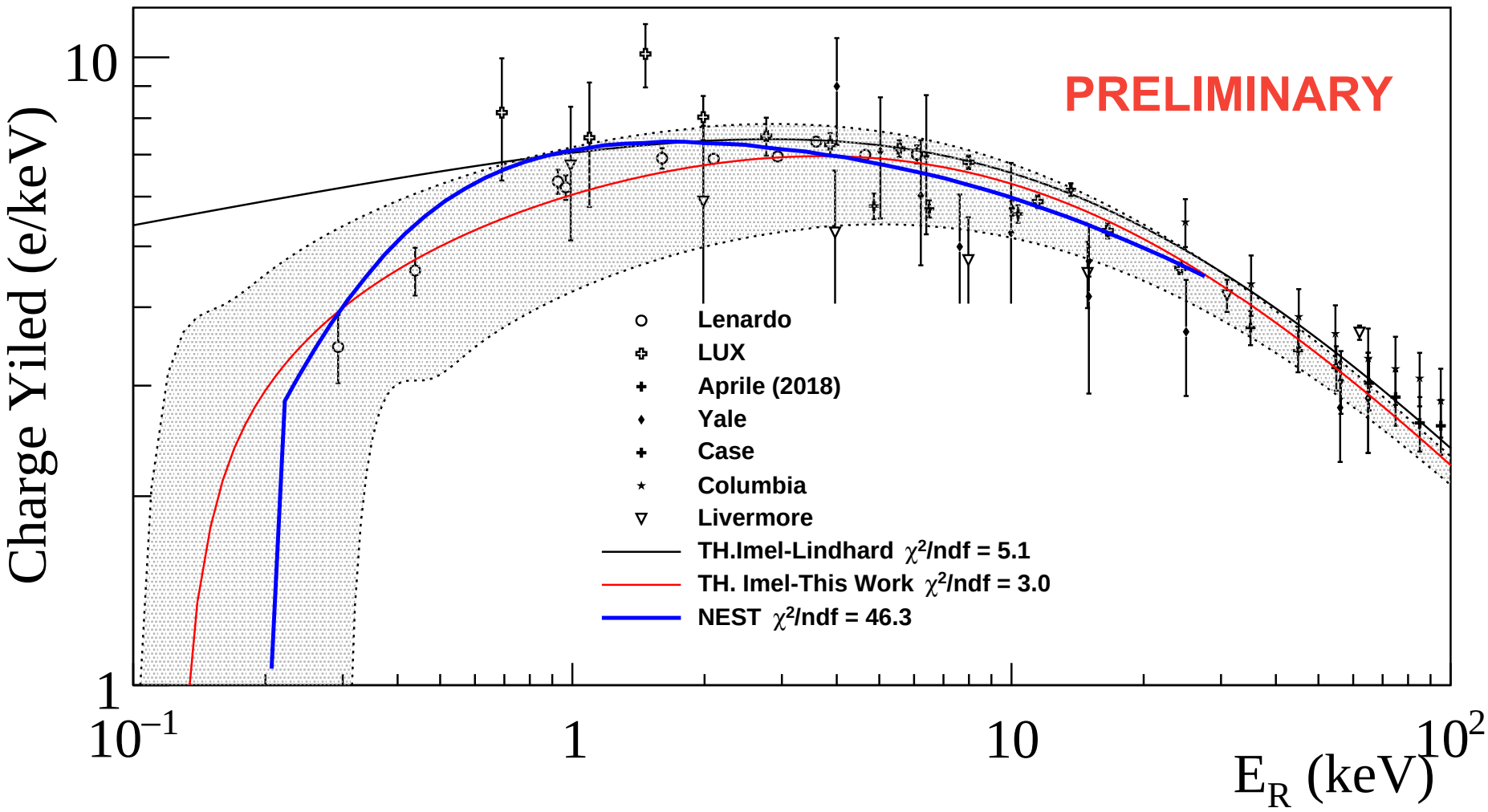


Figure: Charge Yield for Xe; $N_{ext}/N_i = 0.42$ and $\gamma = 0.015$

Xenon Light Yield

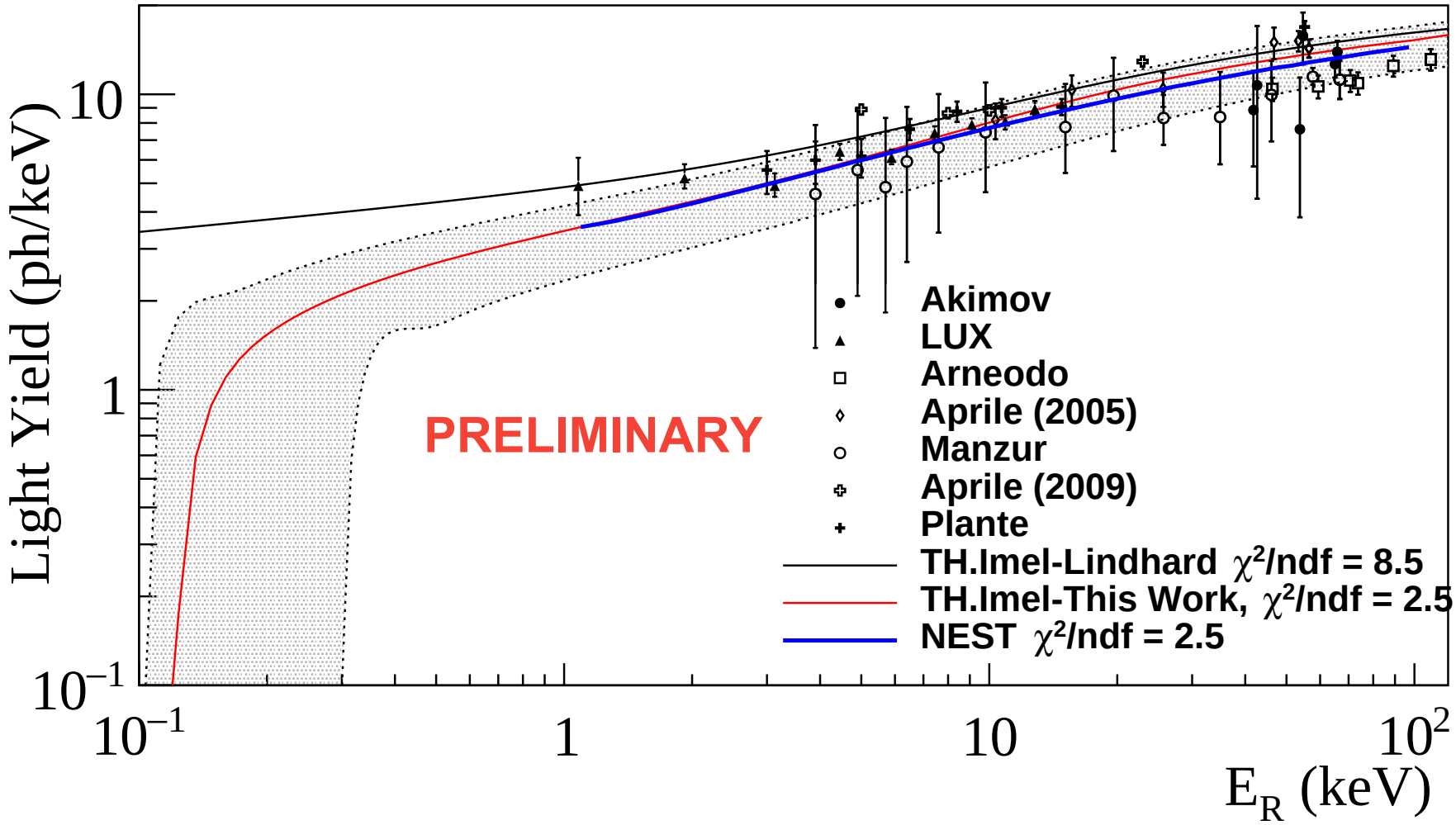


Figure: Light Yield for Xe; $N_{ext}/N_i = 0.42$ and $\gamma = 0.015$

Argon Charge Yield

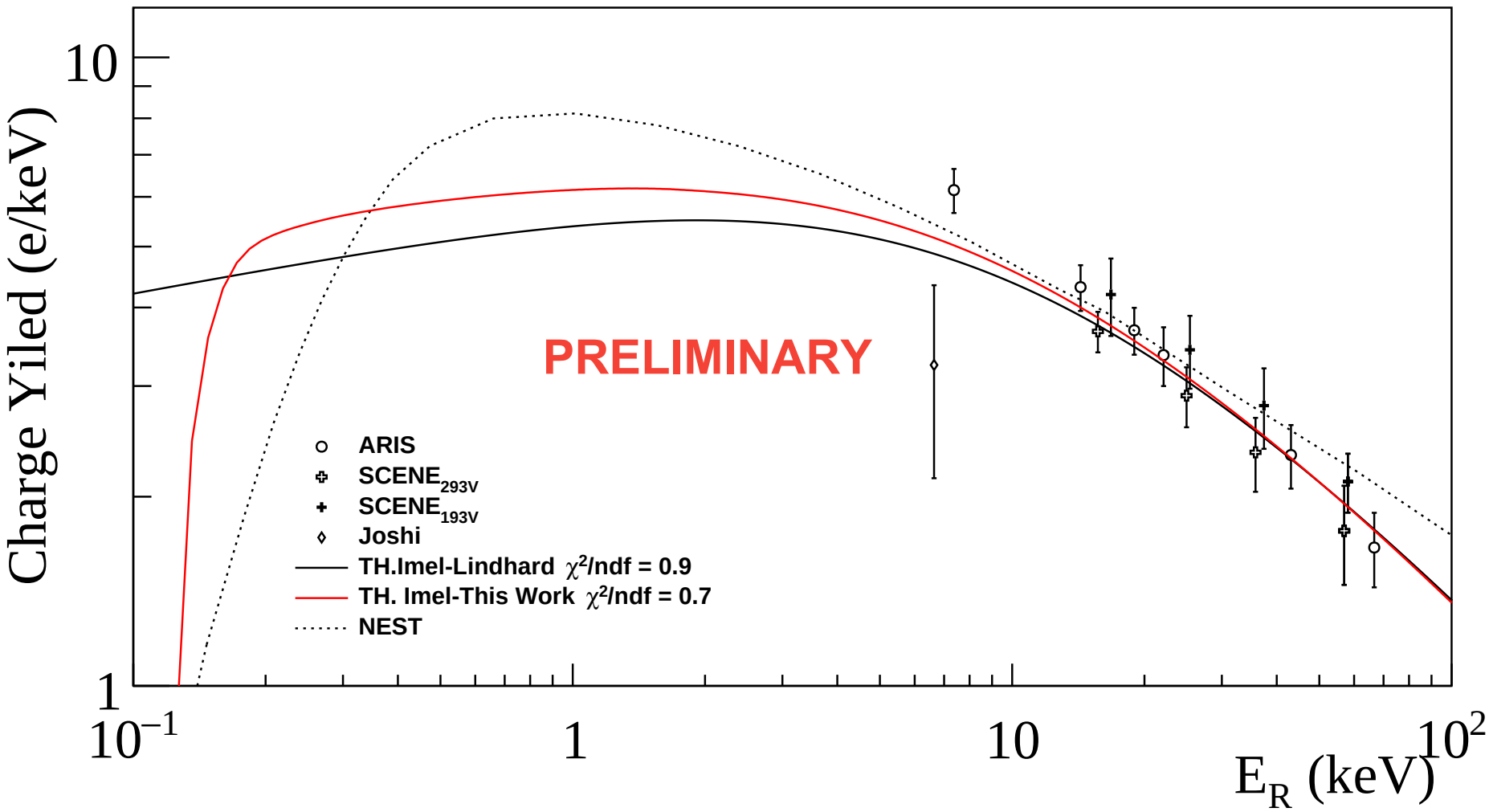


Figure: Charge Yield for Xe; $N_{ext}/N_i = 1.04$ and $\gamma = 0.030$

Argon Light Yield

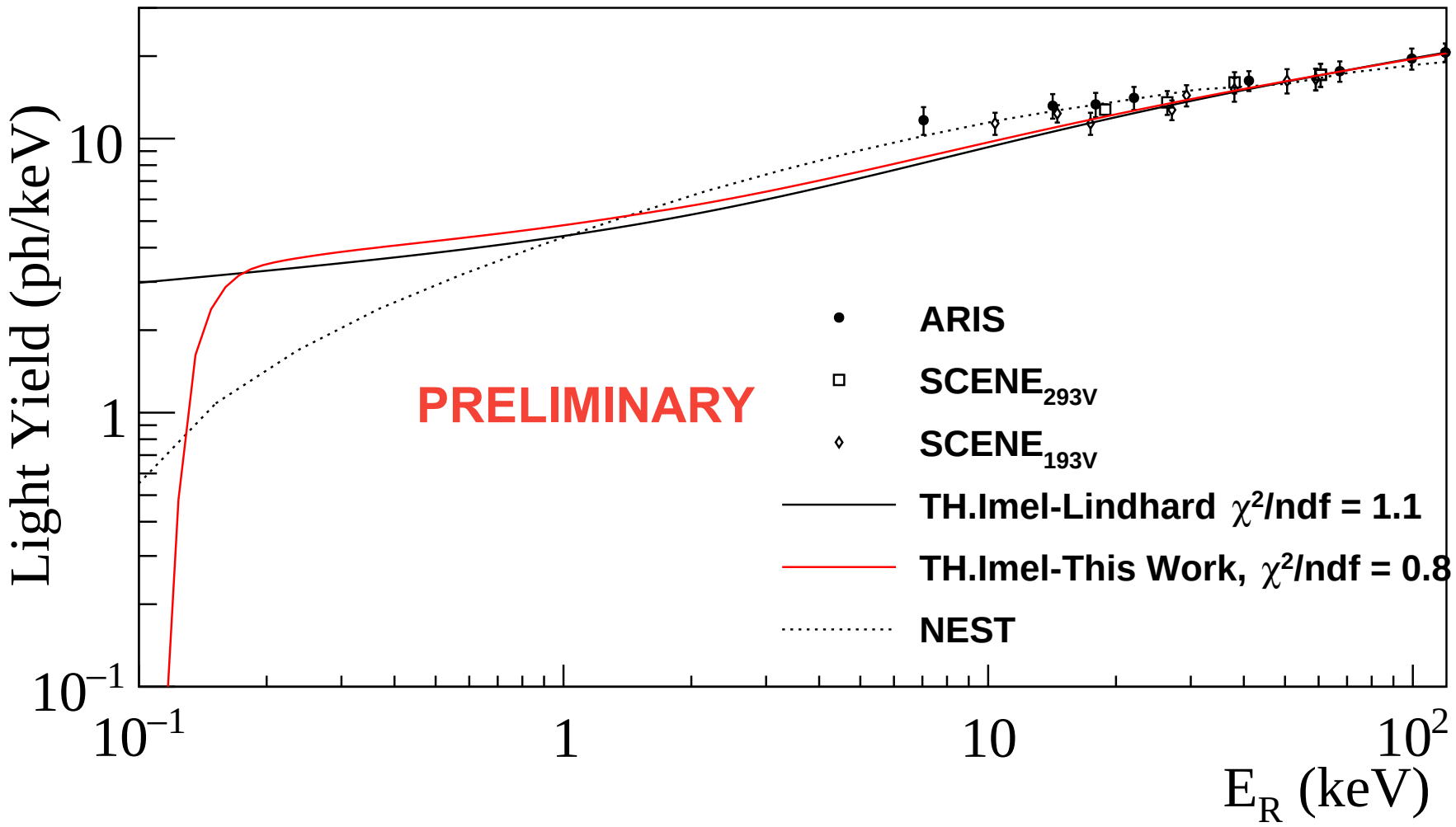


Figure: Light Yield for Xe; $N_{ext}/N_i = 1.04$ and $\gamma = 0.030$

Conclusions

1. *We present a general model based on integral equations for ionization in pure crystals and noble liquids.*
2. *We incorporate corrections due to electronic straggling and atomic scaling in the Int. Diff. Eq.*
3. *For silicon Coulomb effects allow us to fit the data up to 3 MeV and have a threshold near Frenkel-pair creation energy.*

Conclusions

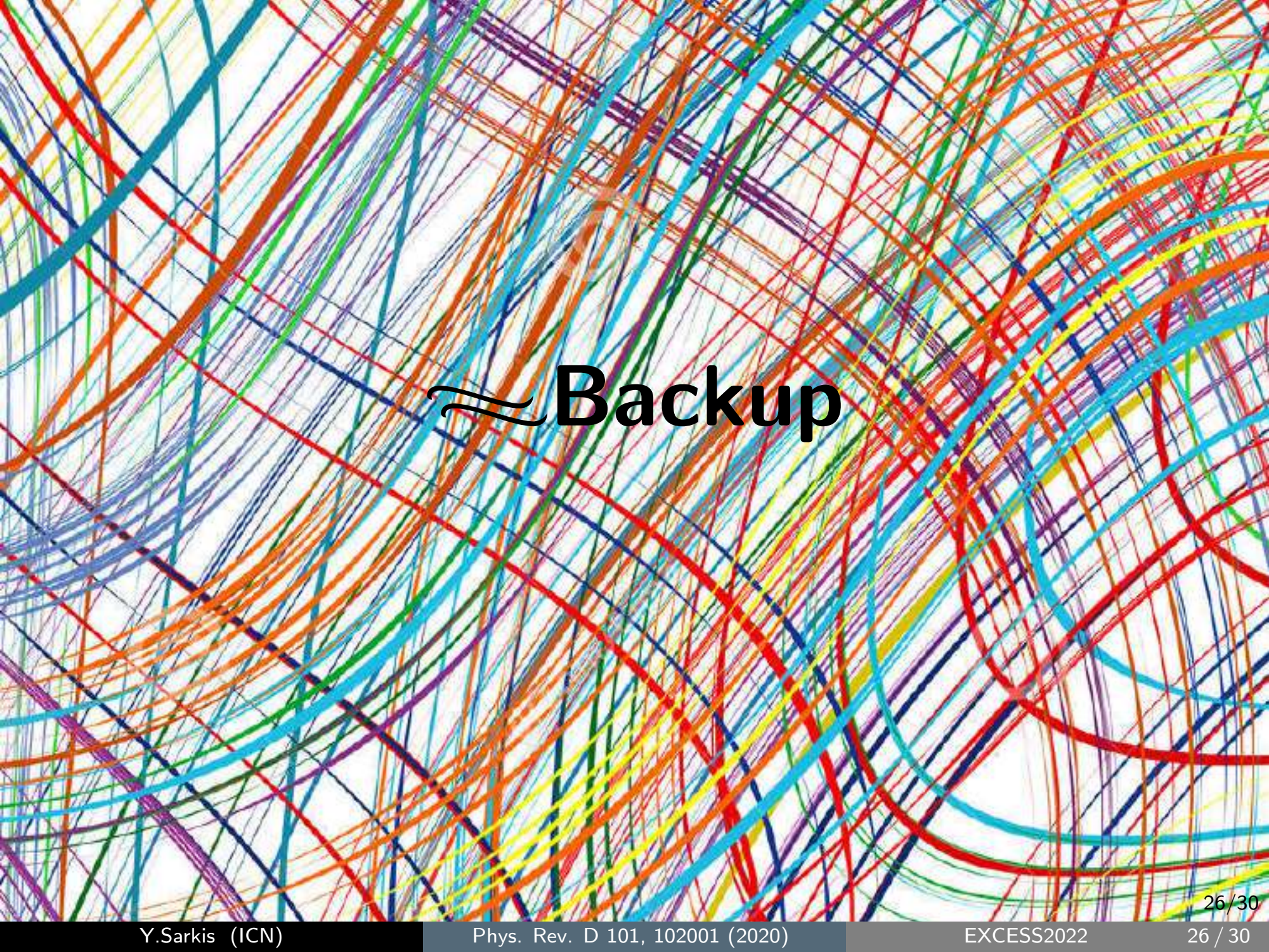
1. *For germanium our model shows potential to explain recent measurements* [5].
2. *We show charge and light yields for Xe and Ar consistent with actual data.*
3. *Much work can be done from here, e.g directional quenching factor, straggling for* $\bar{\nu}$*, etc.*

[5] J.I.Collar, et al, PRD 103,122003 (2021)

Thanks

youssef@ciencias.unam.mx

- *We thank Daniel Baxter for his time and joyfully disposition for presenting this work.*
- *This research was supported in part by DGAPA-UNAM grant number PAPIIT-IT100420, and Consejo Nacional de Ciencia y Tecnología (CONACYT) through gran CB2014/240666.*


Backup

Tilinin geometrical factor

Tilinin argue that for non small angles or a general trajectory of the ion there should exist a geometrical factor: $d\chi\rho d\rho dz' = \left[1 + \left(f_z'(\theta)\right)^2\right]^{1/2} d\chi\rho d\rho dz$. Tilinin made a raw approximation to evaluate the angle

$$\theta \sim Z_1 Z_2 \left(Z_1^{2/3} + Z_2^{2/3}\right)^{-1/2} \left(2e^2/a_0\right)/E,$$

with $\theta < 1$. Is full fill when the energy is $E < 67$ eV for Si and for Ge $E < 190$ eV. As expected for Si the limit is very reasonable and in the order of magnitude of the binding and Tilinin model can be justified to be use.

Many experiments that rely on quenching factors

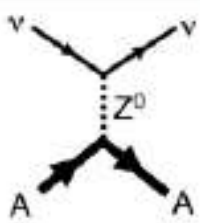
Ge

Liquid scintillators (Xe and Ar)

Si

The RED-100 experiment

Coherent Captain-Mills (CCM) Experiment



CAPSAIN = "Cryogenic Apparatus for Precision Tests of Argon Interactions with Neutrinos"

Low energy effects for electron gas (Scaling)

- Density Functional Theory (DFT) is used to estimate S_e and U.
- Usually the average Fermi energy $\frac{3}{5}E_F$ is associated for electron kinetic energy.
- This assumption is valid only at high energies.
- For low energies [6], due to Pauli exclusion principle, just electrons near E_F could be excited.
- Changing $\frac{3}{5}E_F \to E_F$ in DFT, implies scaling $a = 0.885a_0/Z^{1/3}$ by $\frac{5}{3}$.
- With this $S_e \to \xi_e S_e$, $\xi_e = (5/3)^{3/2}$. **Hence for a wide range of energies ξ_e can vary among 1.0 and $(5/3)^{3/2} \approx$ 2.15.**
- Lindhard added $\xi_e \approx Z^{1/6}$ to explain experimental data[7].
- Now we can understand the origin for ξ_e from DFT as a consequence of considering Pauli principle. Scaling also affects U and W.

[6] I. S. Tilinin Phys. Rev. A 51, 3058, 1 April 1995

[7] Included in the Lindhard formula for k $= 0.133Z^{2/3}A^{-1/2} = 0.133\xi_e(Z/A)^{-1/2}$.

QF with CDMS data