

# Investigating Ultra-Low Energy Ionization Yield from Nuclear Recoils in Semiconductor Detectors via Molecular Dynamics Simulations

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On behalf of CDEX-SCU group

# ► **Low-energy Nuclear Recoil and Ionization Quenching**

► Molecular Dynamic Methods

► Results and Roadmap for Silicon and Germanium

► Impact on Dark Matter Searches

► Summary and Future Prospects

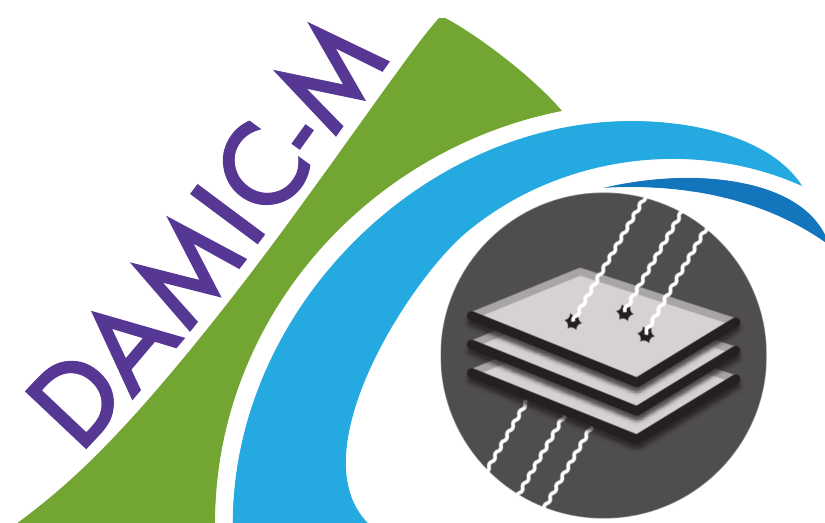


# Low-energy Nuclear Recoil Channel in Particle Physics

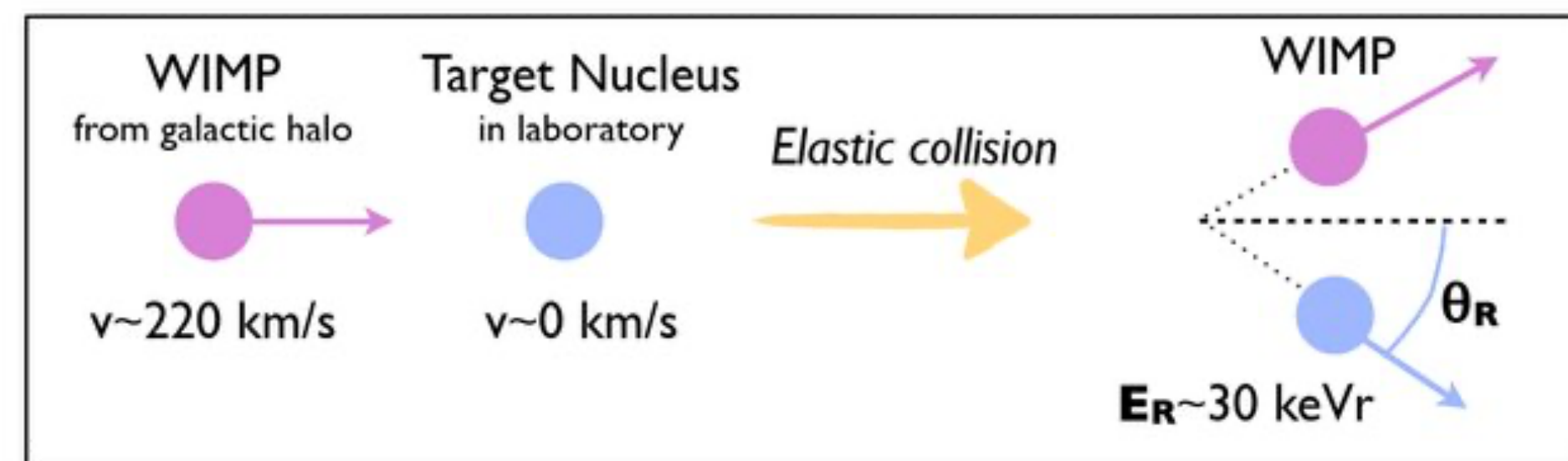
Si



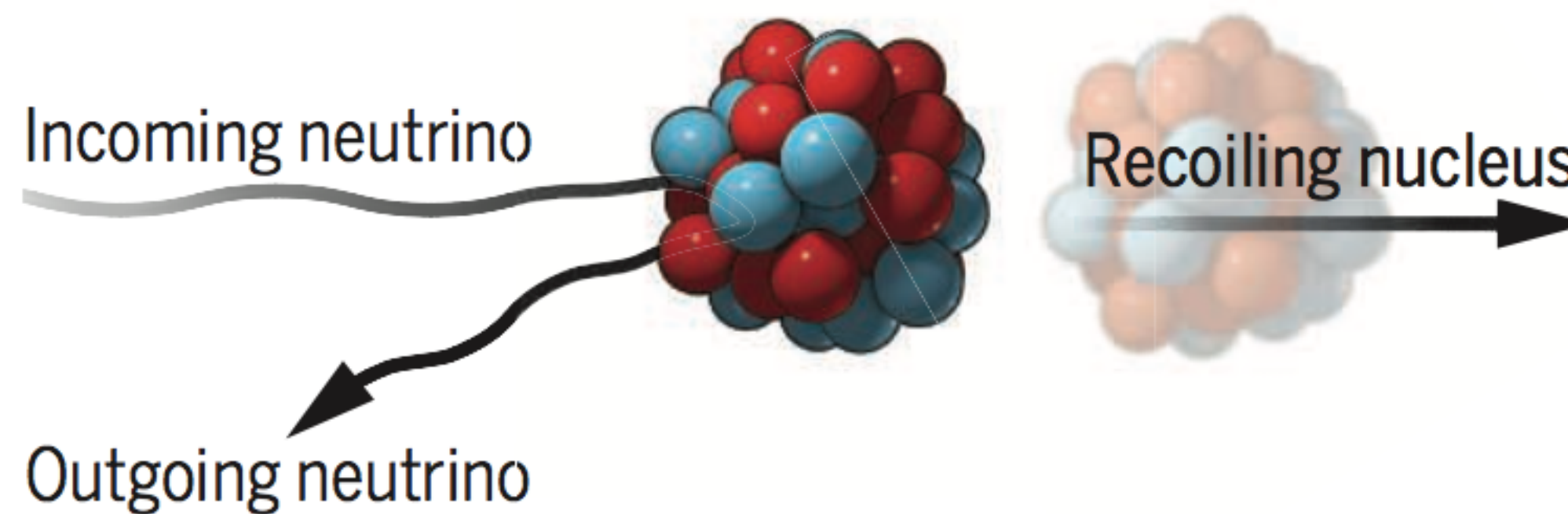
co.vnie  
COHERENT NEUTRINO NUCLEUS  
INTERACTION EXPERIMENT



Etc.



$\chi$ -N scattering

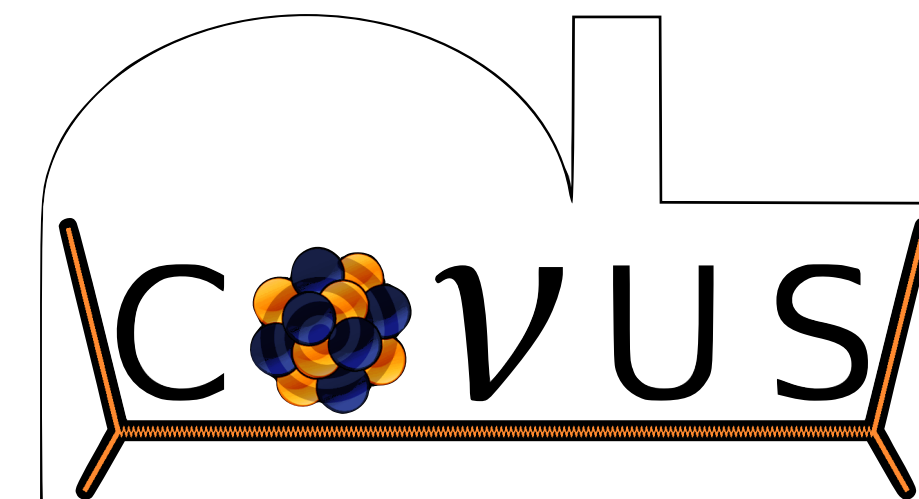


Coherent Elastic neutrino Nuclear Scattering (CEvNS)

Ge



中国暗物质实验  
China Dark matter Experiment



Etc.

# Ionization Quenching on Low-energy Nuclear Recoil

Ionization Quenching Factor (QF)

(< 1)

$$E_{ee} = Q \times E_{nr}$$

Measured  
Energy

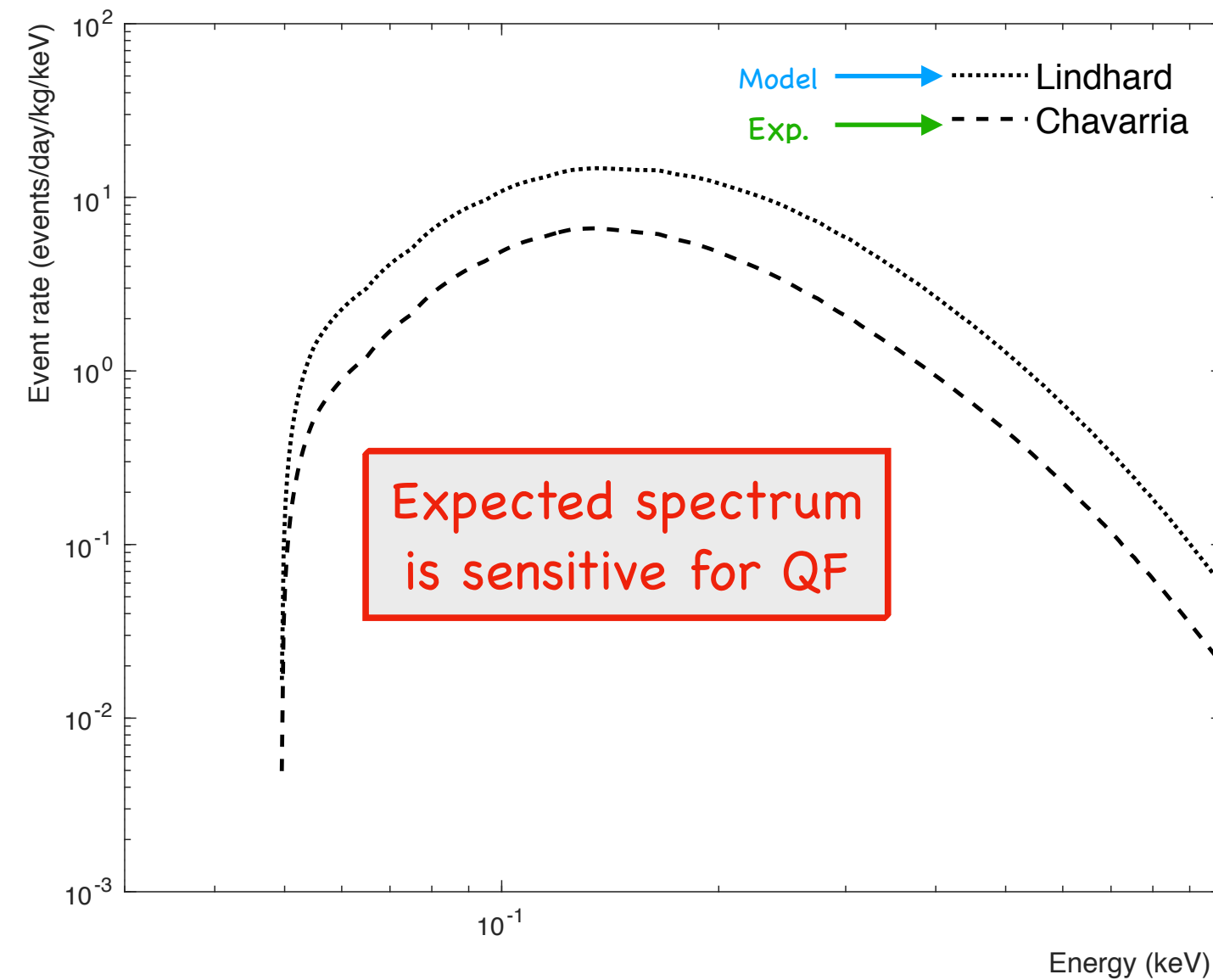
Nucl. Recoil  
Energy

Detector Ionization Response

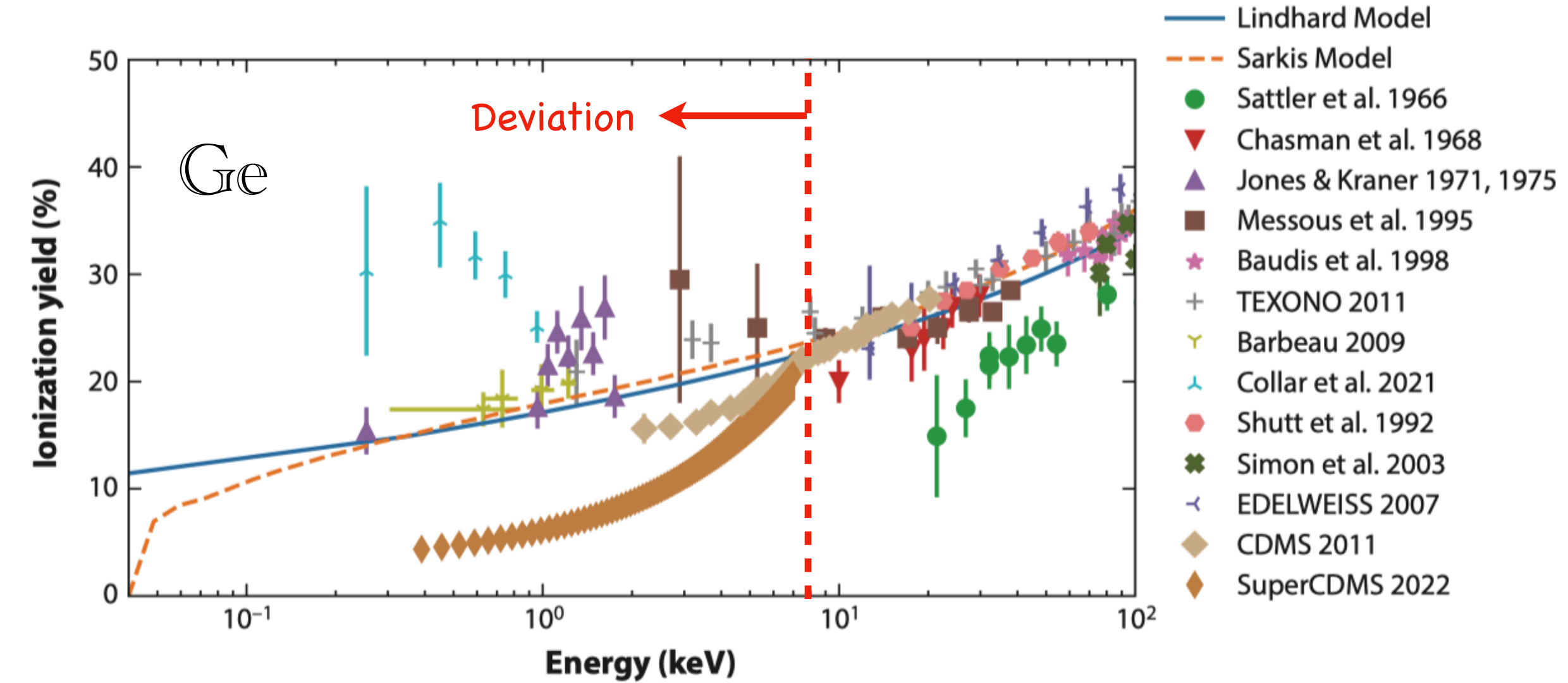
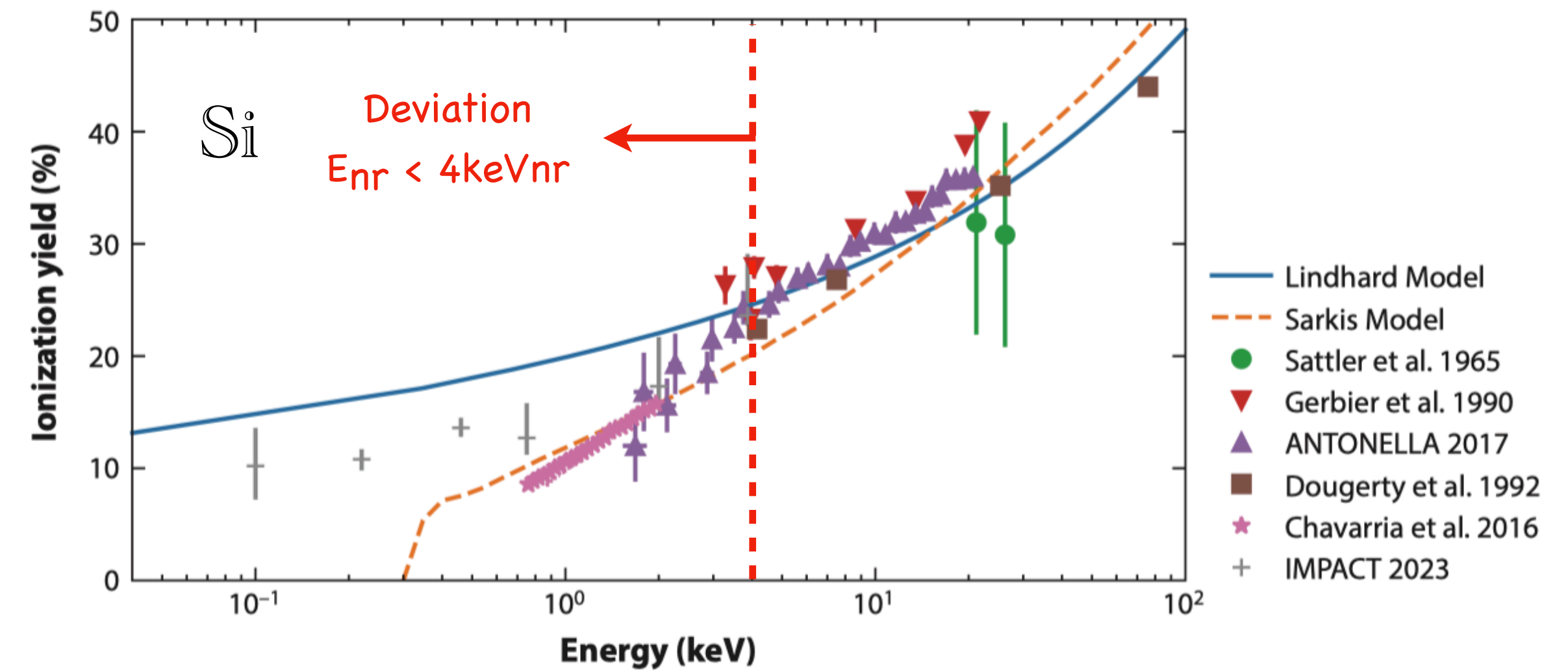
$$\frac{dR}{dE_{ee}} = \frac{dR}{dE_{nr}} \frac{1}{Q} \left( 1 + \frac{E_{nr}}{Q} \frac{dQ}{dE_{nr}} \right)^{-1}$$

Exp.  
Spectrum

Theoretical  
Spectrum



CEvNS's expected event rate dependence on QF. [CONNIE2019]



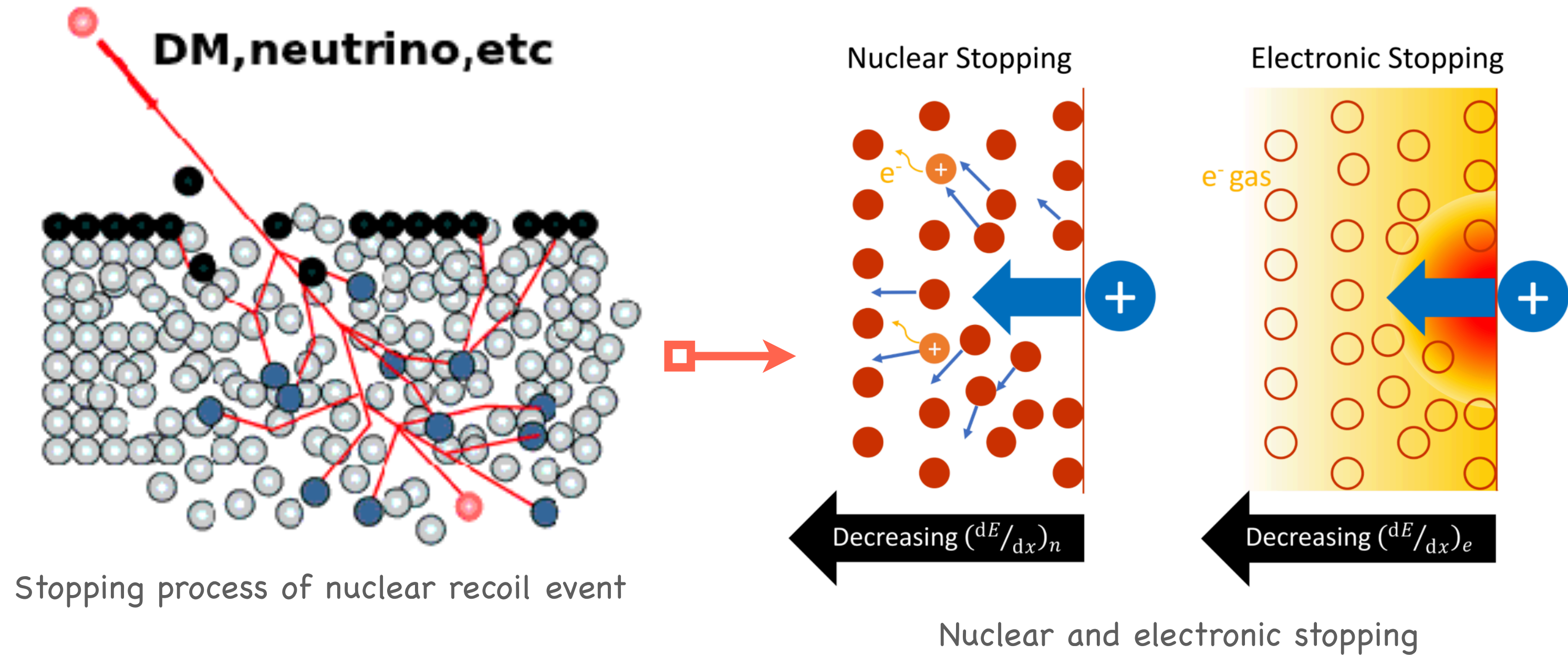
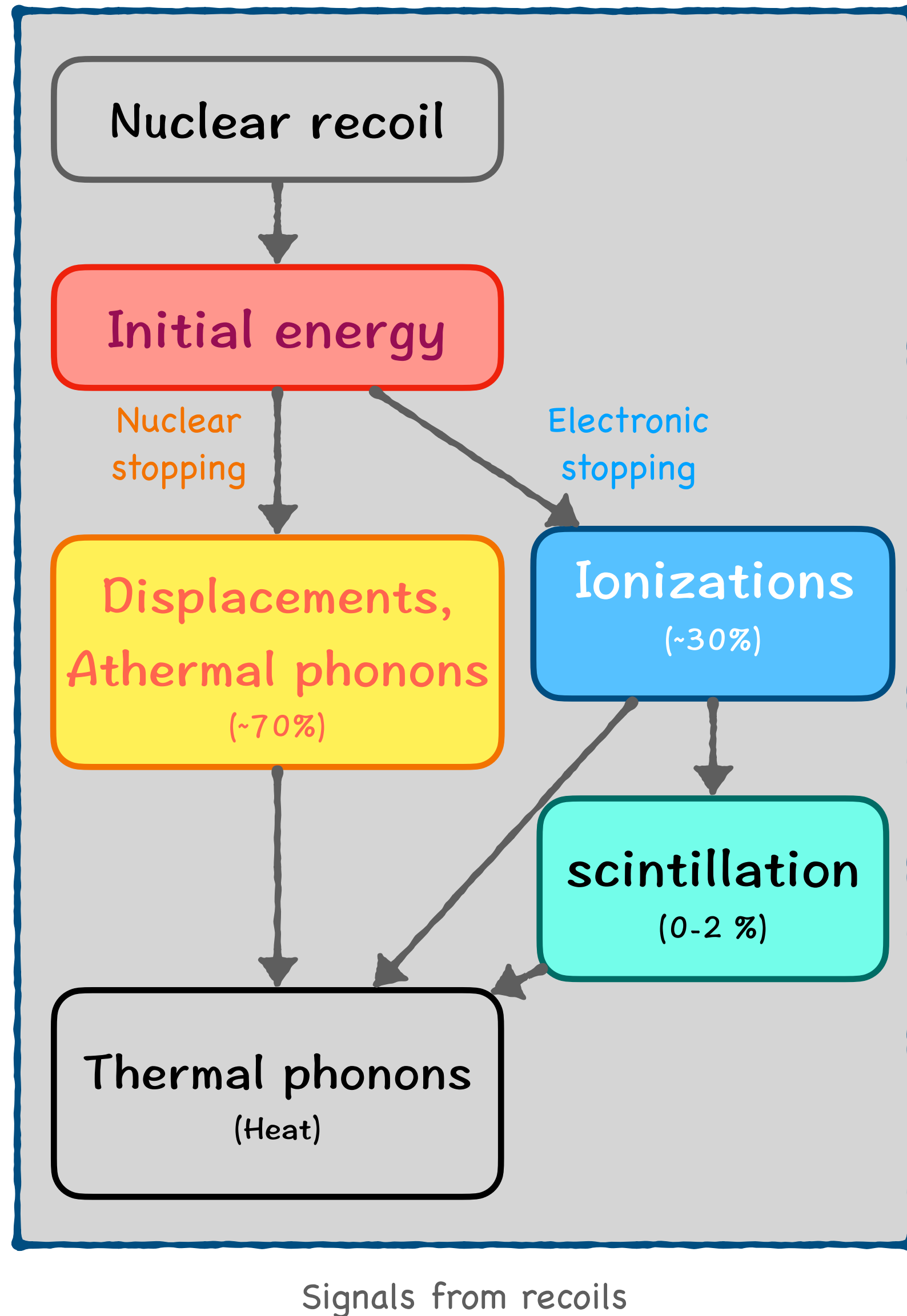
Ionization yields of Si (top) and Ge (bottom) measurements [1].

- QFs are unavoidable detector response for ionization/scintillation detection.
- A considerable source of uncertainty for physical results interpretation.



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# Picture of Ionization Quenching



- Competition of energy loss process: **Nucl.** vs. **Elec.**
- Picture of quenching: Nucl. Recoil energy → Displacements, Vibrations + **Ionization (visible energy)**.



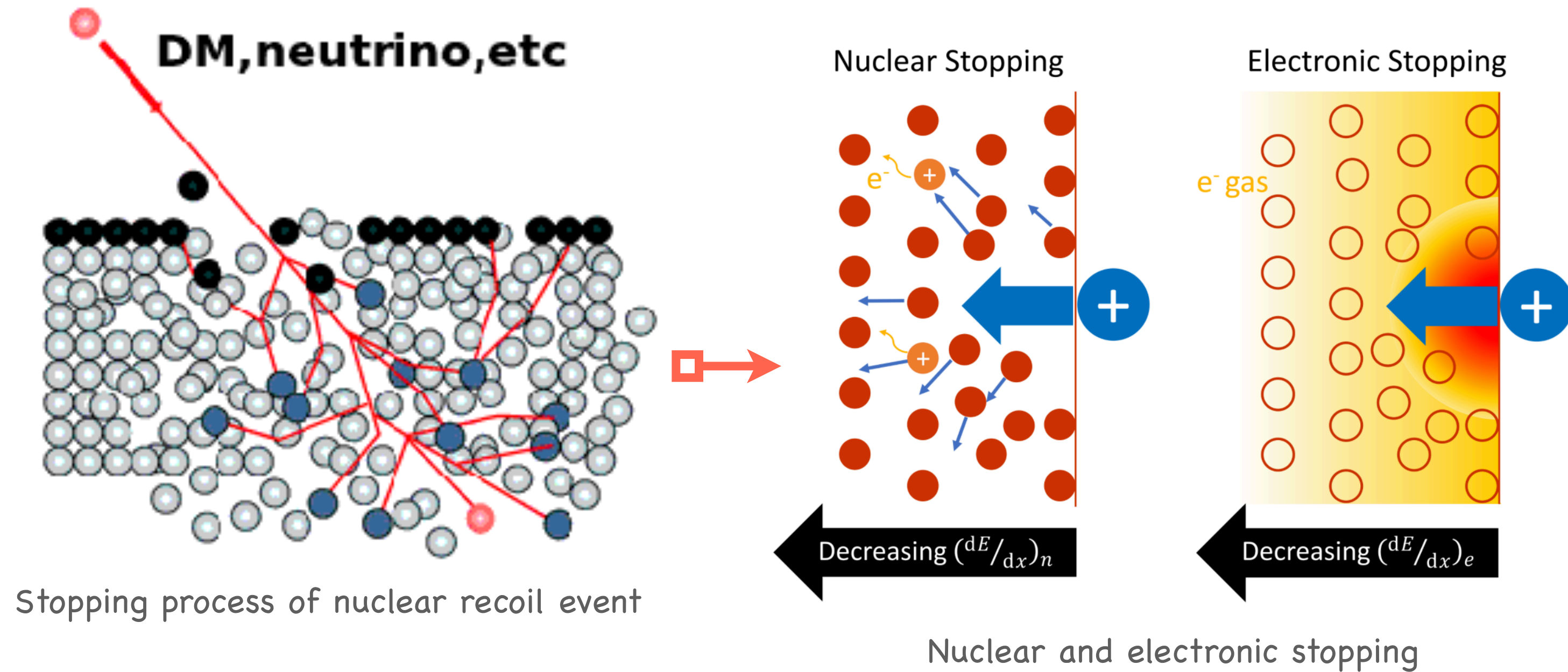
# Molecular Dynamics Approach

$$Q = E_{ee}/E_{nr}$$

## Lindhard's (five) approximations

- I Neglect contribution to atomic motion coming from electrons.
- II **Neglect the binding energy,  $U = 0$ .**
- III The energy transferred to ionized electrons is small compared to that transferred to recoiling ions.
- IV Effects of electronic and atomic collisions can be treated separately.
- V  $T_n$  is also small compared to the energy  $E$ .

Expected to be valid for sufficiently high energies.

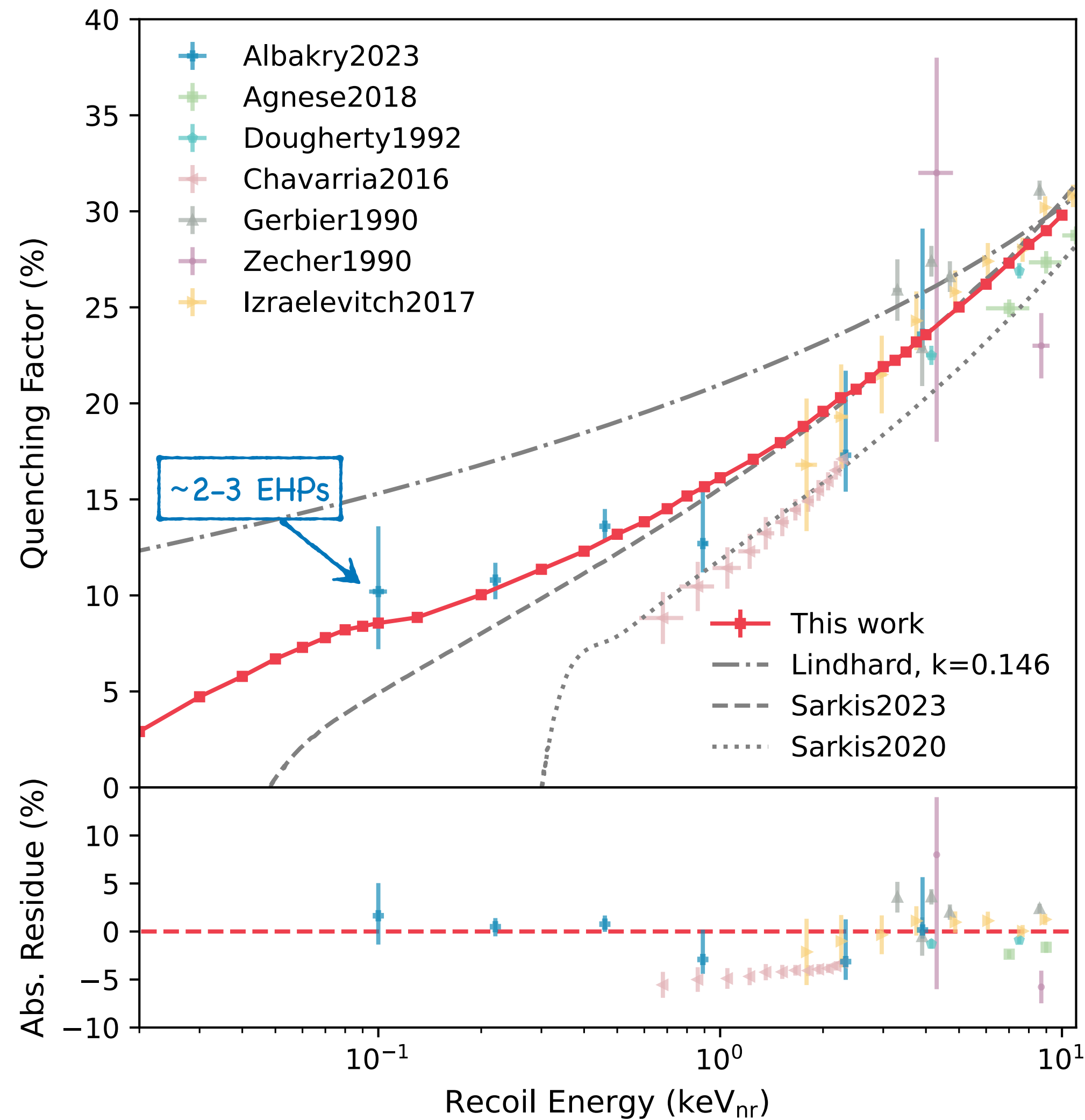


- Intuitively models energy allocation to ionization during nuclear recoil transport.
- Naturally incorporates **highly anisotropic lattice binding** and **structure** into atomic collision processes. (Beyond Lindhard model)

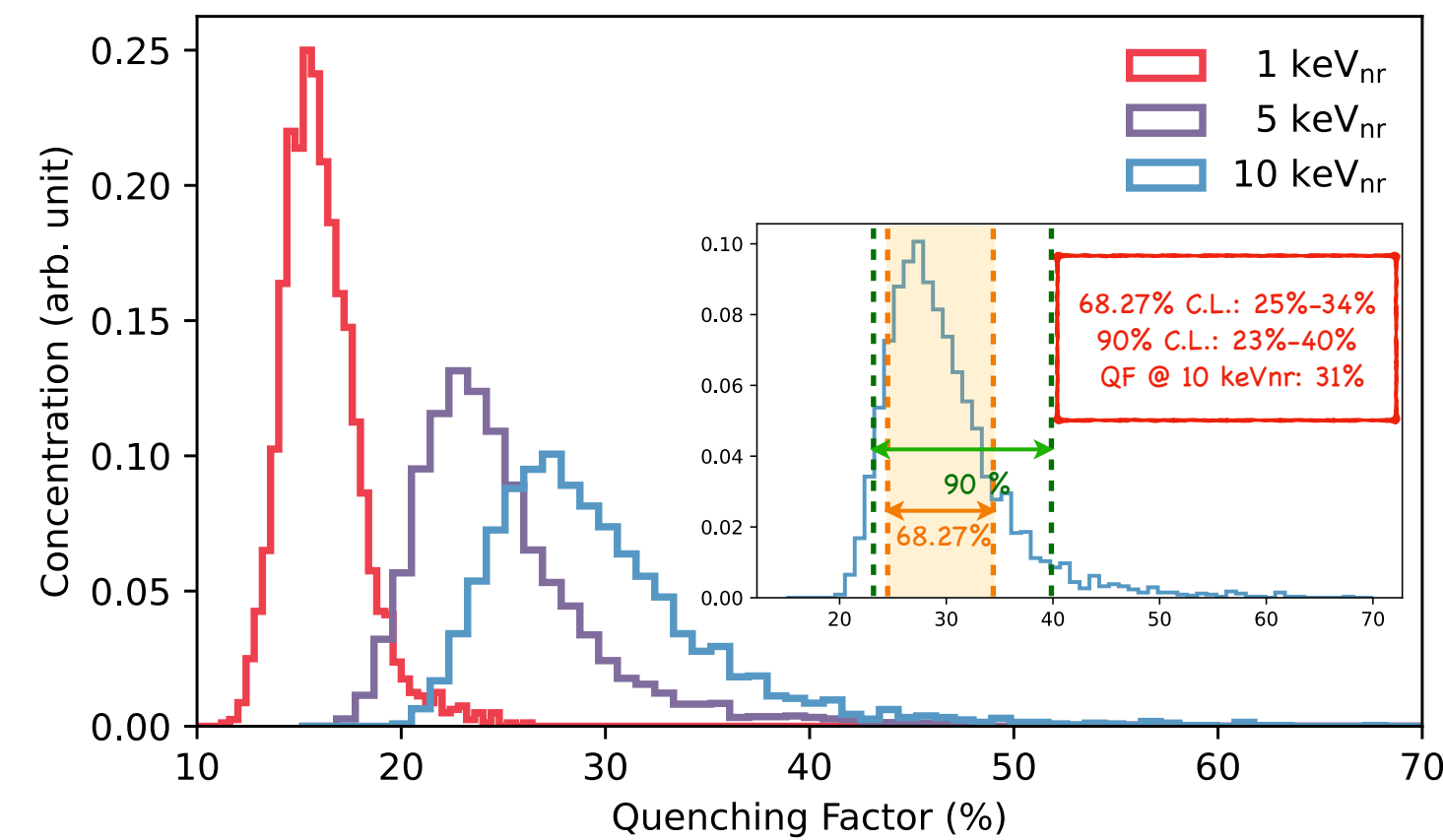
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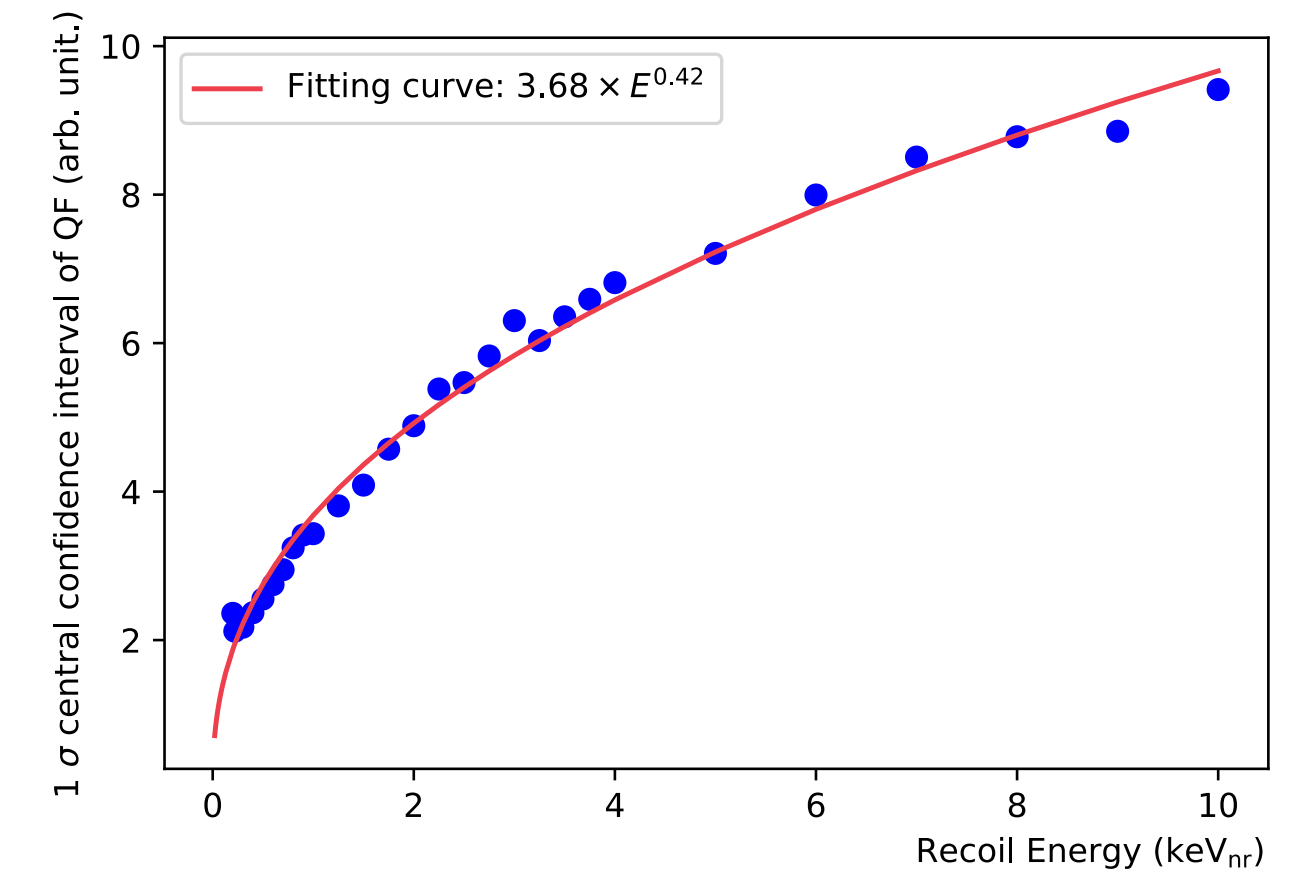
# Ionization yield and Its Randomness of Silicon



Calculated mean value of Si QFs compared to measurements and the Lindhard-like models.



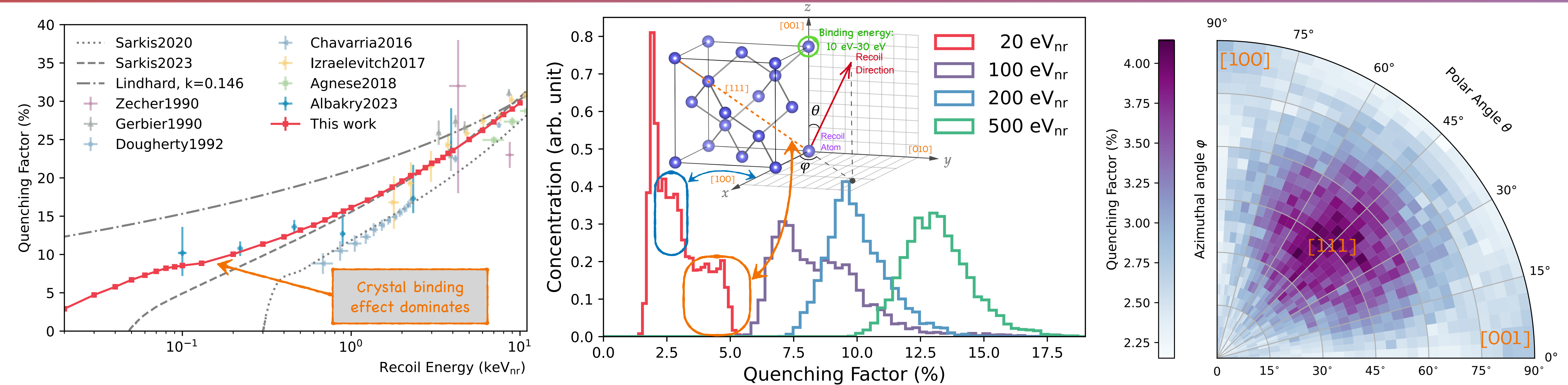
Distribution of QFs for keV scale recoil events.



1 $\sigma$  width of ionization distribution as function of recoil energy (> 200 eV<sub>nr</sub>).

- The results demonstrate a **high consistency** with the measurements, even at **the scale of a single electron-hole pair (EHP)**.
- Inherent distribution of QFs originates from the random cascade process.
- The broad distribution of QF values indicates that using mean values is **insufficient**.

# Lattice structure and Low-energy behavior



QF of calculations and measurements.

Distribution of QFs for sub-keV scale recoil events.

Recoil angular dependence of the QF at 20  $\text{eV}_{\text{nr}}$ , showing mean QF over  $(\theta, \phi)$ .

- **Above 10  $\text{keV}_{\text{nr}}$**  (not shown): Consistence with Lindhard and Sarkis model, indicates binding is not important.
- **From 200  $\text{eV}_{\text{nr}}$  to 10  $\text{keV}_{\text{nr}}$** : Address overestimation of Lindhard model via neglecting binding effect, but no special structure in distribution.
- **Below 200  $\text{eV}_{\text{nr}}$** : Lattice binding dominates the QF behavior.



# Ionization Yield of Germanium

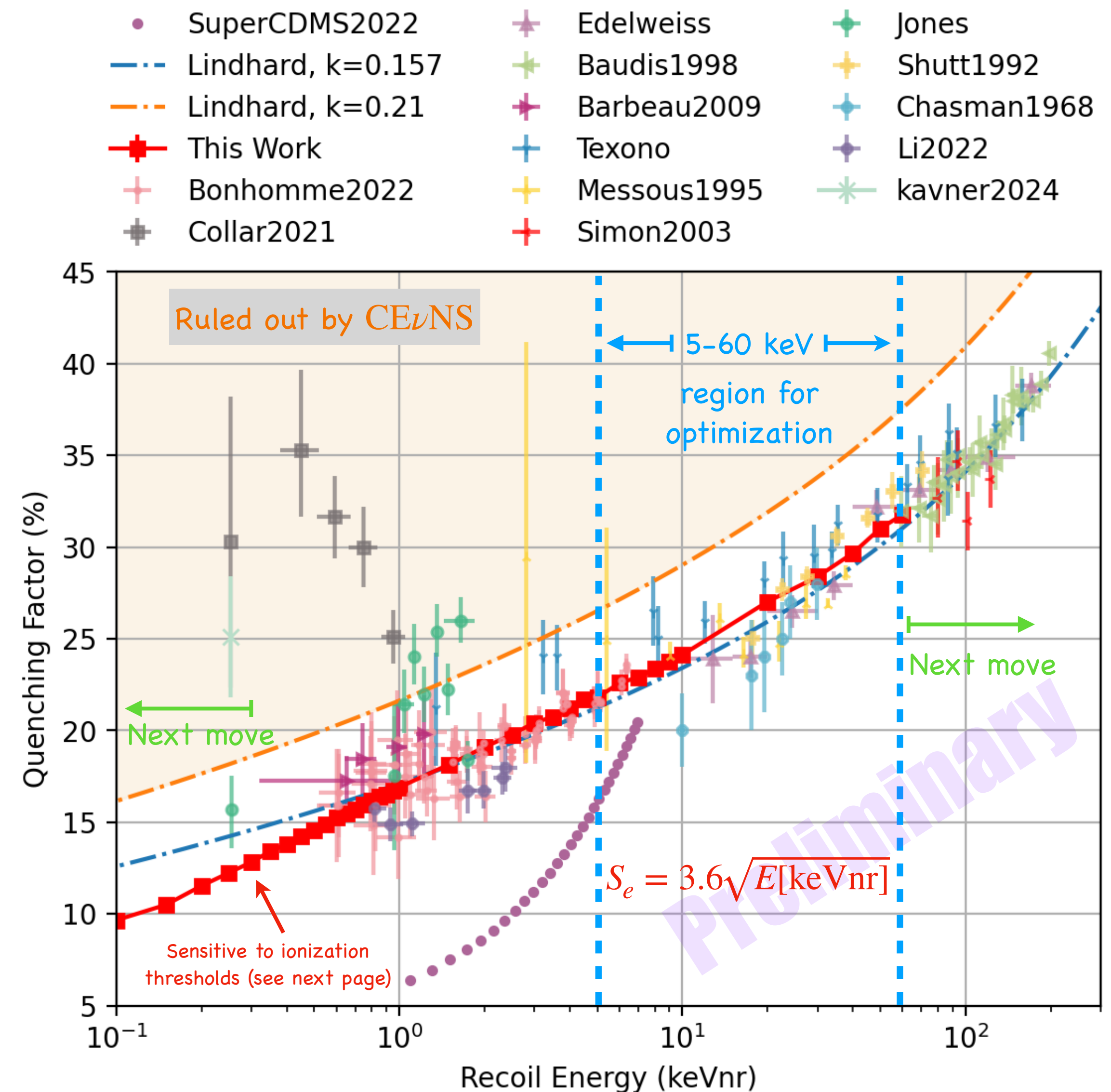
$$\chi^2 = \frac{(y - f(x))^2}{ey^2 + (\frac{1}{2}(exl + exh)f'(x))^2}$$

$$S_e = a\sqrt{E} \quad (v < 1\alpha c)$$

	Chi-square	NDF
Texono2009	12.70	9
baudis1998	0.05	1
EDELWEISS	11.07	5
messous1995	44.85	8
shutt1992	17.84	6
bonhomme2022	6.04	8
chasman1968	7.89	6
TOTAL	100.45	43

Chi-square of optimized k for recoil energy from 5 to 60 keVnr.

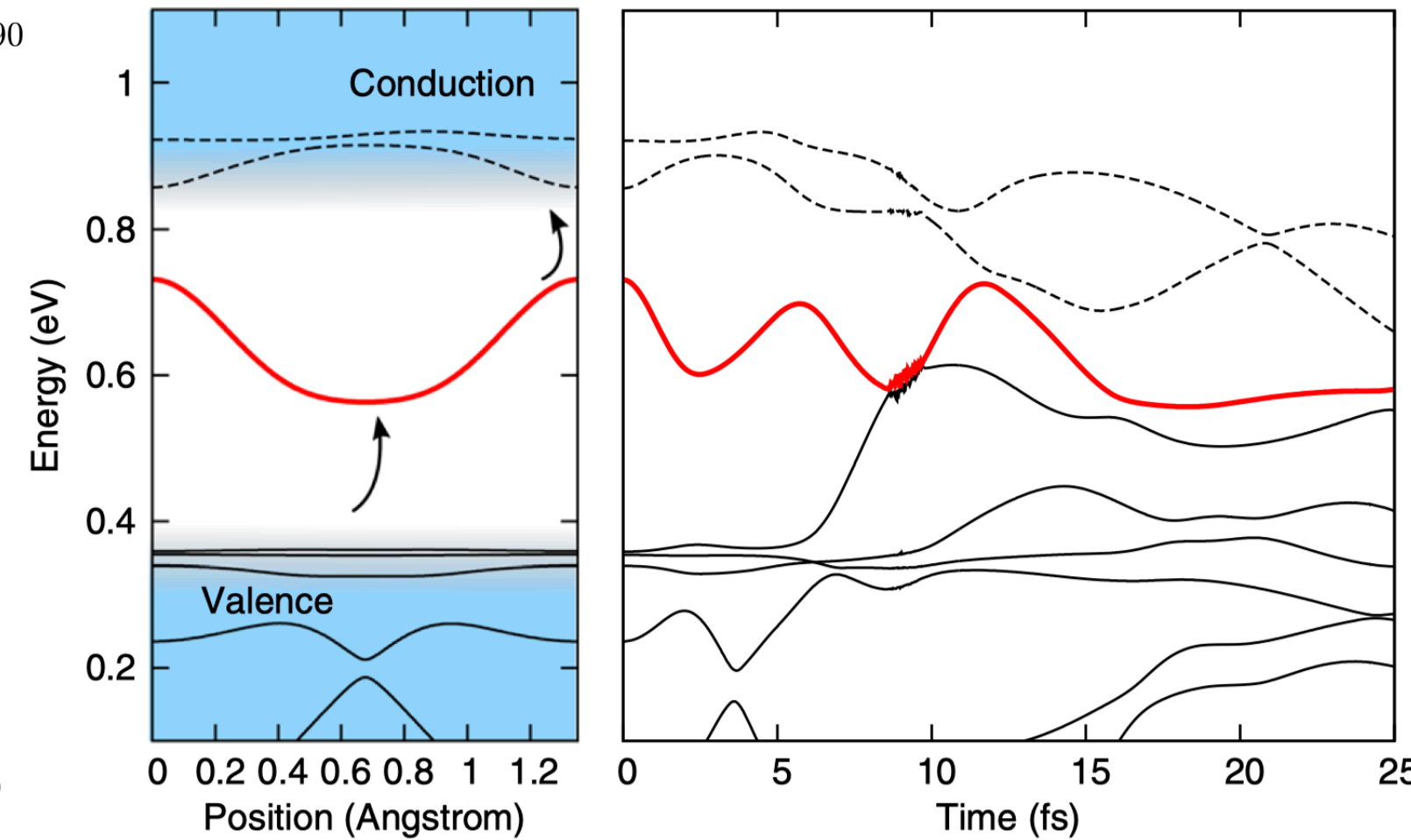
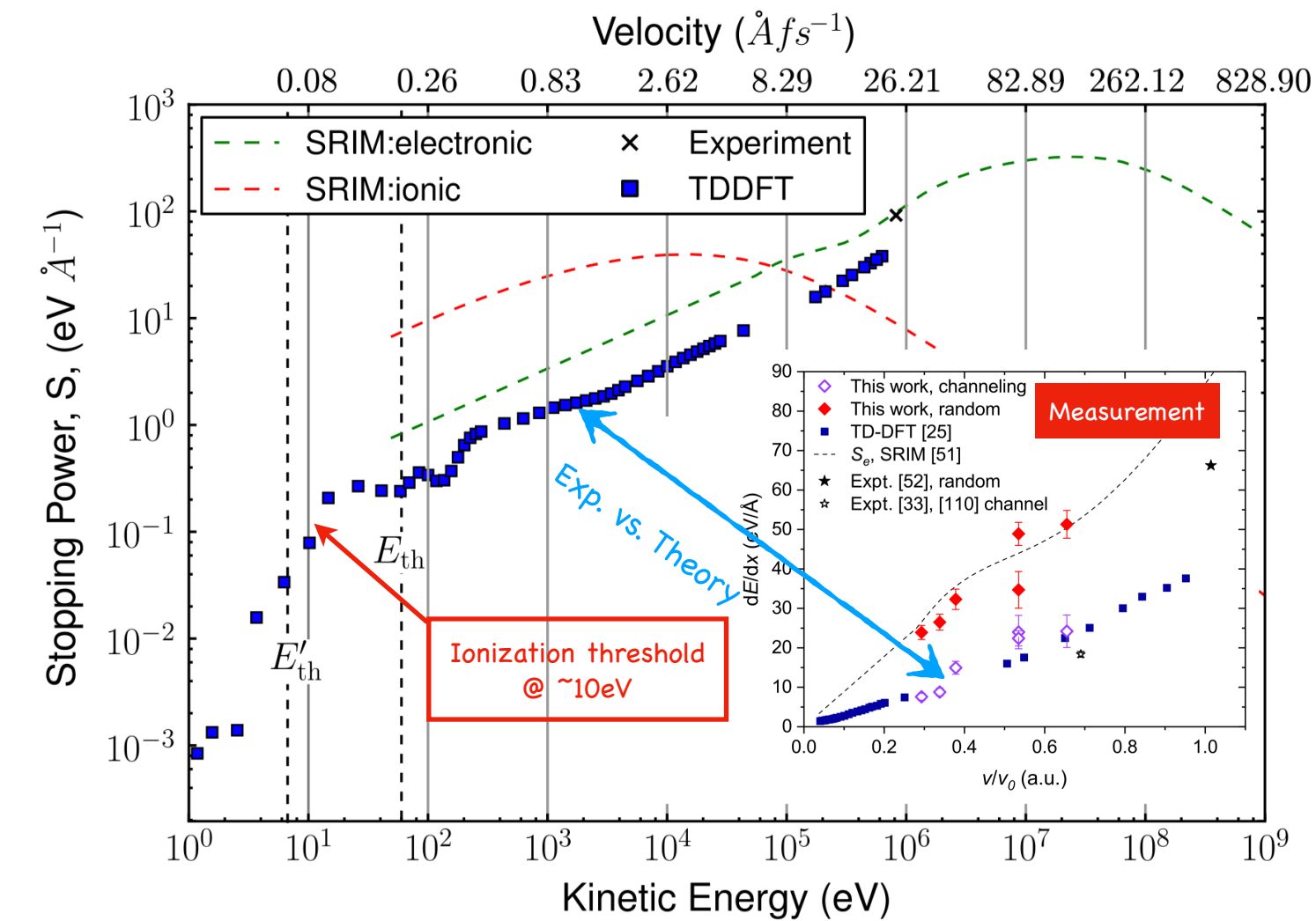
- Binary Search: Optimize the scale factor  $a$  of  $S_e$  with 7 groups, 43 measurements.
- Extending to high-energy: aligns with the Lindhard model and measurements.
- Consistence with most measurements, but Collar and Kavner's measurements.



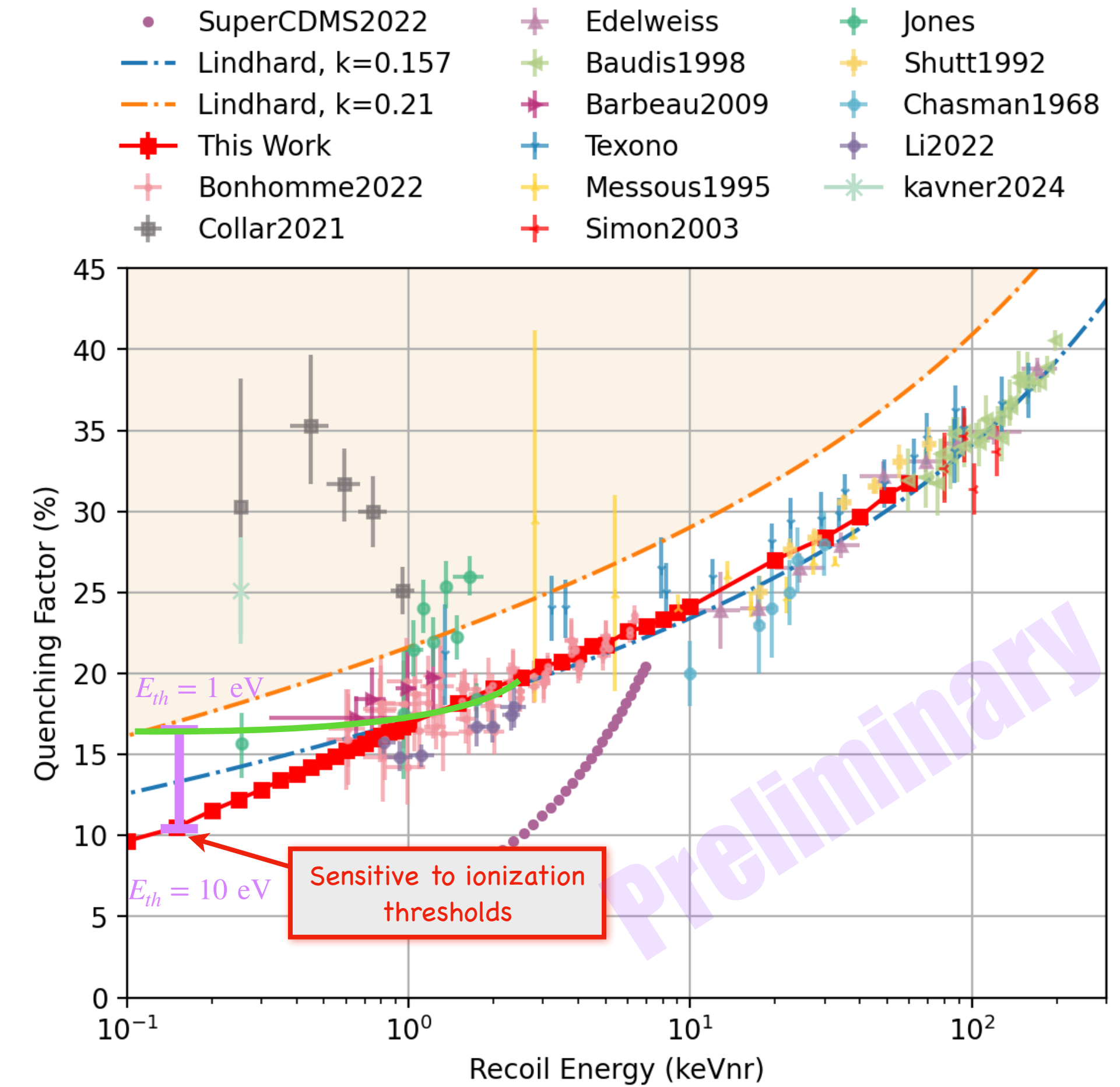
Calculated QF compared to measurements of Ge and the Lindhard models with different parameters. Shadow region is not supported by recent CEvNS results [1-4]

[1] N. Ackermann et al., Direct observation of coherent elastic antineutrino-nucleus scattering, Nature 643, 1229 (2025)  
[2] N. Ackermann et al., Final CONUS Results on Coherent Elastic Neutrino-Nucleus Scattering at the Brokdorf Reactor, Phys. Rev. Lett. 133, 251802 (2024)  
[3] I. Alekseev et al., First results of the  $\nu$ GeN experiment on coherent elastic neutrino-nucleus scattering, Phys. Rev. D 106, L051101 (2022)  
[4] J. Liao, H. Liu, and D. Marfatia, Implications of the first evidence for coherent elastic scattering of reactor neutrinos, Phys. Rev. D 106, L031702 (2022)

# Limitation of Ionization Yield of Nuclear Recoil



The time evolution of mid-gap elevator state (red) as the projectile moves in the crystal [1].



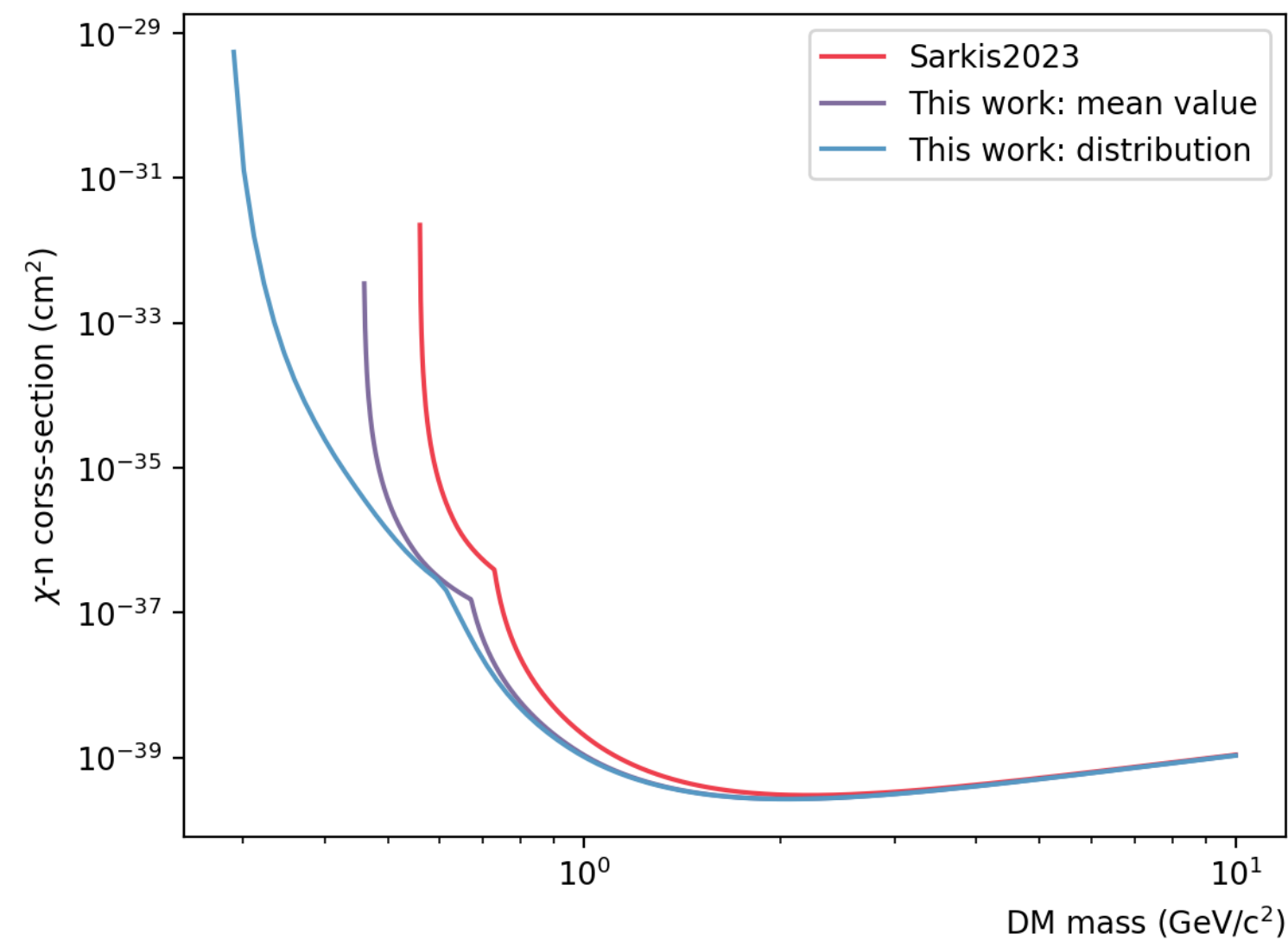
- Ionization threshold ( $E_{th}$ ) is identified through **ab initio** calculations [1, 2] and experiments [3].
- Incorporating **band-gap effects** into the nuclear-electron interactions is crucial for QF calculation **below ~1 keVnr**.
- **Cross-check** with previously optimized  $S_e$ .
- Ab initio calculation for  $S_e$  of germanium is **on-going**.

[1] Lim, A. et al. Electron Elevator: Excitations across the Band Gap via a Dynamical Gap State. Phys. Rev. Lett. 116, 043201 (2016).  
 [2] Lohmann, S., Holeňák, R. & Primetzhofer, D. Trajectory-dependent electronic excitations by light and heavy ions around and below the Bohr velocity. Phys. Rev. A 102, 062803 (2020).  
 [3] Roth, D. et al. Electronic Stopping of Slow Protons in Oxides: Scaling Properties. Phys. Rev. Lett. 119, 163401 (2017).

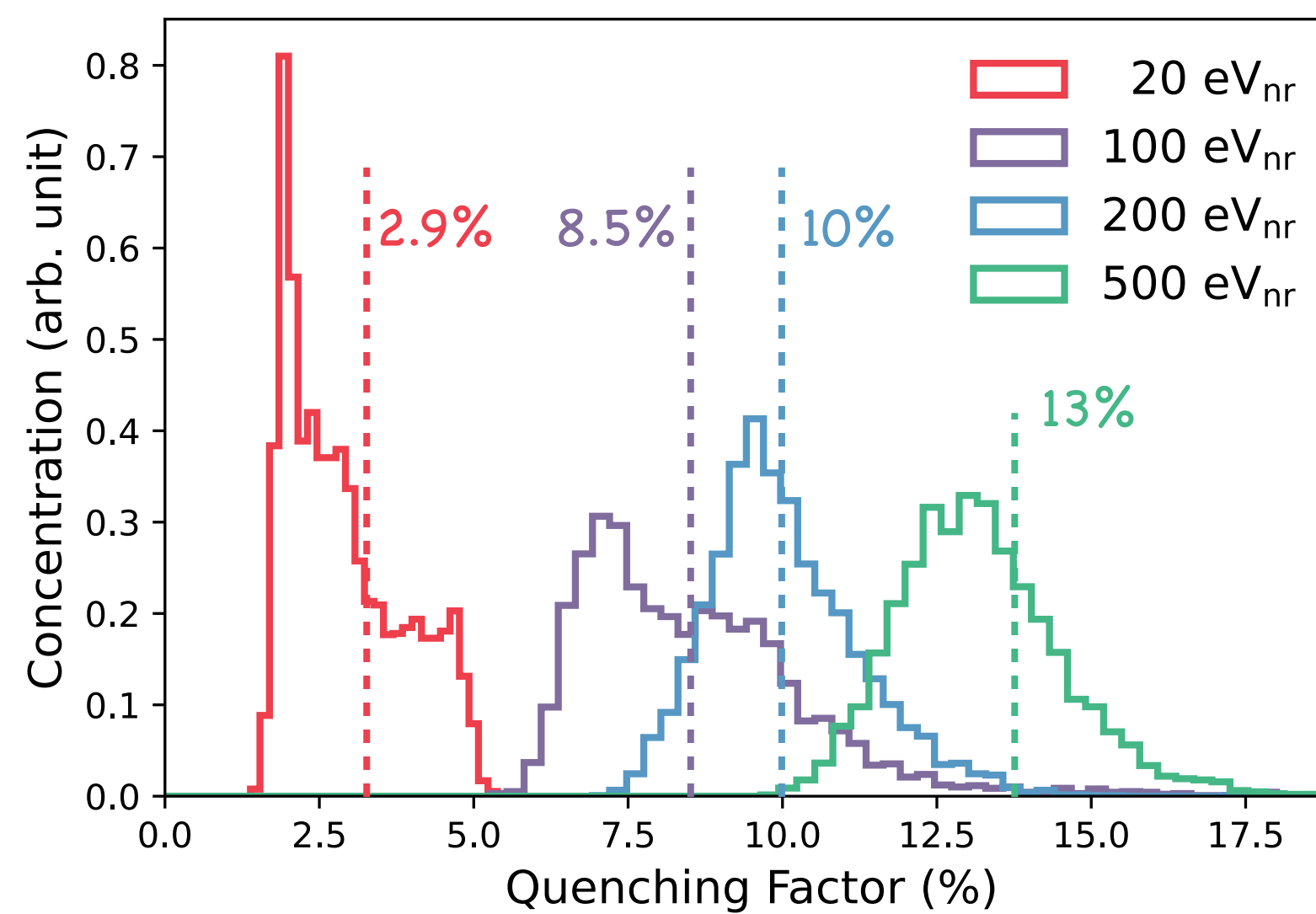


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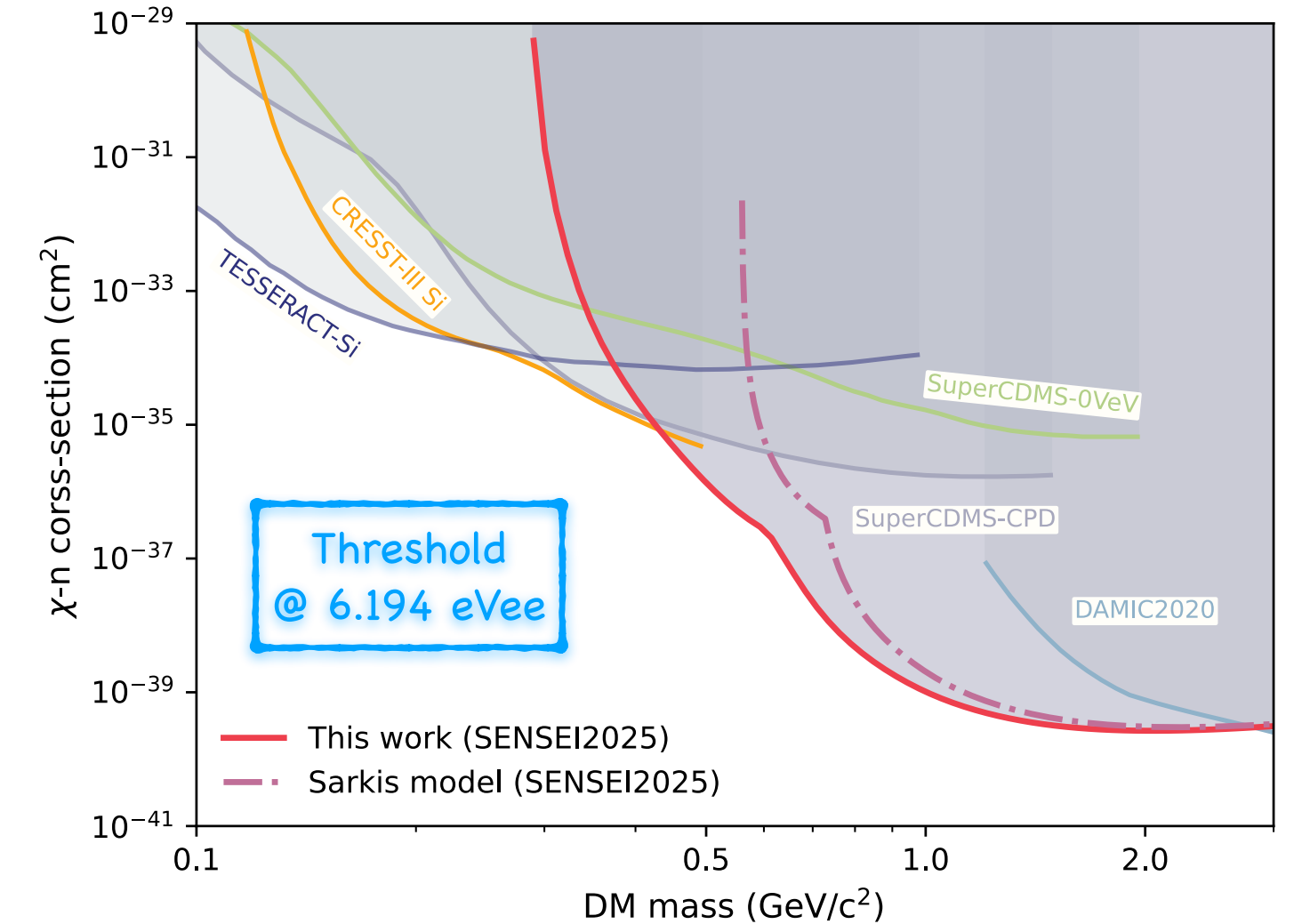
# Re-interpretation for sub-GeV Dark Matter Constrains



90% C.L. exclusion limits from SENSEI-2025 via three different QF treatments.



Low-energy events leak to higher Electronic equivalent energy via QF distributions.



90% C.L. upper limits for the  $\chi$ -N interaction reinterpreted from SENSEI spectrum

- Reinterpreted of **SENSEI-2025 (6.194 eVee)** [1] with **Sarkis model**, **MD-calculated mean QF**, **MD-calculated full QF distribution** using binned Poisson method.
- Standard DM Halo parameters:  $v_{\text{esc}} = 544$  km/s,  $v_0 = 220$  km/s,  $\rho_{\text{DM}} = 0.3$  GeV/cm<sup>3</sup>/c<sup>2</sup>
- Convolution with QF distribution: **Enhance sub-GeV constrain**, **extended exclusion limit to 0.29 GeV/c<sup>2</sup>**.



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# Summary and Prospects

## Summary

- Develop a **novel** method to evaluate QFs. Demonstrates good agreement with measurements in silicon even at the **level of a single electron-hole pair**.
- Considerable width of QF distribution indicating using mean values is **insufficient**. From the distribution perspective constrain on sub-GeV dark matter is **extended and enhanced**.

## Prospects

- Calculation for Germanium still requires more acknowledgement of electronic stopping power, **especially for ionization limitation raised by band gaps**.
- Confirm the QF distribution with experiments.
- The distribution of the QF might be **universal** in ionization/scintillation detection, as it originates from the random cascade process.



Thank you for your attention!